Science Supplementary Material
SM358 The Quantum World

SM358

Additional Exercises for Book 1

Contents

This set of exercises relates to Book 1 of SM358 and can be used for further practice and for revision purposes. To gain maximum benefit, it is important to attempt each question for yourself before looking up the solution.

Exercises

Topic 1 — de Broglie waves

Exercise 1.1 A one-dimensional de Broglie wave describing a free particle takes the form

$$\Psi_{\rm dB}(x,t) = e^{i(Ax-Bt)},$$

where $A = 3.20 \times 10^{10}\,\mathrm{m}^{-1}$, $B = 7.44 \times 10^{14}\,\mathrm{s}^{-1}$ and the potential energy is equal to zero everywhere.

(a) What are the wave number, angular frequency, wavelength and period of this wave?

(b) What are the momentum magnitude, kinetic energy and mass of the particle?

Exercise 1.2 Show that the one-dimensional de Broglie wave function

$$\Psi_{\rm dB}(x,t) = e^{2\pi i(x/\lambda - t/T)},$$

where λ and T are positive constants, is an eigenfunction of the momentum operator $\widehat{\mathrm{p}}_x$, and find the corresponding eigenvalue. Is your answer consistent with the de Broglie relation linking the magnitude of momentum to the wavelength of a free particle?

Topic 2 — Operators

Exercise 2.1 Determine whether each of the following operators is linear:

$$\widehat{\mathrm{O}}_1 f(x) = x^2 f(x)$$

$$\widehat{\mathrm{O}}_2 f(x) = f^2(x)$$

$$\widehat{\mathrm{O}}_3 f(x) = f(x+a),$$

where a is a constant, and $f(x)$ is an arbitrary function. Explain your reasoning.

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Exercise 2.2 Simplify the expression

$$\left(\widehat{\mathrm{O}}_1\widehat{\mathrm{O}}_2 - \widehat{\mathrm{O}}_2\widehat{\mathrm{O}}_1\right)g(x)$$

where the operators $\widehat{\mathrm{O}}_1$ and $\widehat{\mathrm{O}}_2$ are defined by

$$\widehat{\mathrm{O}}_1 f(x) = \frac{\mathrm{d}f(x)}{\mathrm{d}x} \quad \text{and} \quad \widehat{\mathrm{O}}_2 f(x) = x^2 f(x)$$

for any function $f(x)$.

Topic 3 — Schrödinger's equation

Exercise 3.1 An isolated one-dimensional system consists of two particles of masses m_1 and m_2 interacting via a potential energy function $\frac{1}{2}C(x_1 - x_2)^2$, where C is a positive constant and x_1 and x_2 are coordinates representing the positions of the particles.

Write down a Hamiltonian function, a Hamiltonian operator and Schrödinger's equation for this system, showing explicitly all the variables and parameters involved.

Exercise 3.2 A one-dimensional system consists of two particles of masses m_1 and m_2, which do not interact with each other, and are each subject to a potential energy function of the form $\frac{1}{2}Cx^2$, where C is a positive constant and x represents position.

Write down a Hamiltonian function, a Hamiltonian operator and Schrödinger's equation for this system, showing explicitly all the variables and parameters involved.

Exercise 3.3 (a) Write down Schrödinger's equation for a free particle of mass m in one dimension and show that the solutions of this equation obey the principle of superposition.

(b) A beam of electrons is incident on an absorbing screen which contains two narrow slits. Some particles in the beam pass through the slits and are detected on a screen on the far side. How does the principle of superposition help to explain the pattern built up by a large number of particles falling on the detecting screen?

Topic 4 — Separation of variables

Exercise 4.1 The one-dimensional form of Schrödinger's equation for a particle of mass m in a potential energy well $V(x)$ is

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t).$$

(a) Use the method of separation of variables to show that solutions to this equation exist in the form $\Psi(x,t) = \psi(x)T(t)$. Derive the equations that $\psi(x)$ and $T(t)$ must satisfy, and solve the equation for $T(t)$.

(b) Can all the solutions of Schrödinger's equation be written in this form? Explain your answer.

Exercise 4.2 The time-independent Schrödinger equation for a particle of mass m inside an infinite three-dimensional square well takes the form

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) = E\psi(x,y,z).$$

Use the method of separation of variables to show that solutions to this equation exist in the form $\psi(x,y,z) = X(x)Y(y)Z(z)$. Derive the equations that $X(x)$, $Y(y)$ and $Z(z)$ must satisfy, and specify a relationship that exists between the constants appearing in these equations.

Topic 5 — Born's rule

Exercise 5.1 (a) State Born's rule for a wave function $\Psi(x,t)$ of a particle in one dimension.

(b) A normalized one-dimensional wave function takes the form

$$\Psi(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\mathrm{e}^{-\mathrm{i}Et/\hbar} \quad \text{for } 0 \leq x \leq L.$$

where L is a length and E is an energy. Estimate the probability that a measurement of the particle's position will give a value in the small interval between $x = 0.249L$ and $x = 0.251L$. Does this probability depend on time?

Exercise 5.2 At time $t = 0$, a particle is in a state described by the normalized wave function

$$\Psi(x,0) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{5\pi x}{L}\right) & \text{for } 0 \leq x \leq L, \\ 0 \quad \text{elsewhere.} \end{cases}$$

What is the probability of finding the particle somewhere between $x = 0$ and $x = L/5$ at $t = 0$?

You may use the standard integral

$$\int_0^\pi \sin^2 u \, \mathrm{d}u = \frac{\pi}{2}.$$

Exercise 5.3 A particle is in the ground state of a one-dimensional finite potential well with walls at $x = -L/2$ and $x = +L/2$. Outside the well, the ground-state energy eigenfunction is

$$\psi_1(x) = \begin{cases} C\mathrm{e}^{-\alpha x} & \text{for } x \geq +L/2, \\ C\mathrm{e}^{+\alpha x} & \text{for } x \leq -L/2. \end{cases}$$

(a) What is the probability of finding the particle somewhere outside the well? Express your answer in terms of C, α and L.

(b) What is the probability of finding the particle somewhere inside the well?

Exercise 5.4 At $t = 0$, a particle is described by a one-dimensional wave function

$$\Psi(x,0) = Ax\,\mathrm{e}^{-x^2/a^2},$$

where A and a are constants. Where is the particle most likely to be found?

Exercise 5.5 (a) Use Born's rule to show that the SI units of a wave function in one dimension are $\mathrm{m}^{-1/2}$.

(b) If a is a length and x is a position coordinate, which of the following functions of x are unsuitable, on dimensional grounds, for representing a one-dimensional wave function at any given instant in time?

(i) $f(x) = \mathrm{e}^{-\pi x^2/2a^2}$

(ii) $g(x) = \sqrt{\dfrac{\pi}{a}}\,\mathrm{e}^{-x^2/2a^2}$

(iii) $h(x) = \sqrt{\dfrac{\pi}{a}}\,\mathrm{e}^{-x^2/2}$.

Topic 6 — Normalization and phase

Exercise 6.1 At $t = 0$, a stationary-state wave function takes the form

$$\Psi(x,0) = A\mathrm{e}^{-x^2/2a^2},$$

where A is a constant and a is a positive constant. Use the normalization condition to find a possible value for A, expressed in terms of a. How much freedom is there in choosing this value?

You may use the standard integral

$$\int_{-\infty}^{\infty} \mathrm{e}^{-u^2/a^2}\,\mathrm{d}u = a\sqrt{\pi} \quad \text{for } a > 0.$$

Exercise 6.2 An unnormalized one-dimensional energy eigenfunction takes the form

$$\phi(x) = \begin{cases} \sin\left(\dfrac{2\pi x}{L}\right) & \text{for } 0 \le x \le L \\ 0 & \text{elsewhere.} \end{cases}$$

Obtain the corresponding normalized eigenfunction (defined up to a phase), explaining your reasoning.

You may use the standard integral

$$\int_0^{n\pi} \sin^2 u \, \mathrm{d}u = \frac{n\pi}{2} \quad \text{for integer } n.$$

Exercise 6.3 An energy eigenfunction for a particle in a three-dimensional infinite square well takes the form

$$\psi(x,y,z) = A\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)\sin\left(\frac{3\pi z}{L}\right)$$

for $0 \le x \le L$, $0 \le y \le L$ and $0 \le z \le L$, with $\psi(x,y,z) = 0$ elsewhere. Find a suitable value of A that ensures that this eigenfunction is normalized. Explain your answer.

You may use the standard integral

$$\int_0^{n\pi} \sin^2 u \, \mathrm{d}u = \frac{n\pi}{2} \quad \text{for integer } n.$$

Exercise 6.4 In this question, ψ_1 and ψ_2 are two different normalized energy eigenfunctions and

$$\psi_\mathrm{A} = \frac{\psi_1 + \mathrm{i}\psi_2}{\sqrt{2}}.$$

Which of the following combinations of ψ_1 and ψ_2 (where α is real) represent exactly the same state as ψ_A?

$$\psi_\mathrm{B} = \frac{\psi_1 - \mathrm{i}\psi_2}{\sqrt{2}}$$

$$\psi_\mathrm{C} = \frac{\mathrm{i}\psi_1 - \psi_2}{\sqrt{2}}$$

$$\psi_\mathrm{D} = \frac{-\mathrm{i}\psi_1 - \psi_2}{\sqrt{2}}$$

$$\psi_\mathrm{E} = \frac{-\mathrm{i}\psi_1 + \psi_2}{\sqrt{2}}$$

$$\psi_\mathrm{F} = \frac{\mathrm{e}^{\mathrm{i}\alpha}\psi_1 + \mathrm{e}^{\mathrm{i}(\alpha+\pi/2)}\psi_2}{\sqrt{2}}$$

$$\psi_\mathrm{G} = \frac{\mathrm{e}^{\mathrm{i}(\alpha-\pi/2)}\psi_1 + \mathrm{e}^{\mathrm{i}\alpha}\psi_2}{\sqrt{2}}.$$

Topic 7 — Square wells

Exercise 7.1 A particle of mass m is in the ground state of a three-dimensional infinite square well which occupies a cubic region with sides of length L. By how much does the energy of this system change if the sides of the cubic box are halved in length to $L/2$, with the particle remaining in the ground state of the new box?

Exercise 7.2 A spinless particle of mass m is in a three-dimensional infinite square well which occupies a cubic region with sides of length L. How many degenerate quantum states correspond to the energy level $E_2 = 3\hbar^2/mL^2$?

Topic 8 — Continuity boundary conditions

Exercise 8.1 Write down continuity boundary conditions for an energy eigenfunction $\psi(x)$ and its derivative $\mathrm{d}\psi/\mathrm{d}x$ at the walls of a one-dimensional finite square well.

In one or two sentences state how the behaviour of an energy eigenfunction at the walls of a finite square well differs from the corresponding behaviour at the walls of an infinite square well.

Exercise 8.2 A particle is in the ground state of a one-dimensional finite square well with walls at $x = -L/2$ and $x = +L/2$. Inside the well the energy eigenfunction describing the particle is

$$\psi_{\text{in}}(x) = A\cos(kx),$$

where A and k are constants. Outside the well, for $x \geq +L/2$, the energy eigenfunction is

$$\psi_{\text{out}}(x) = C\mathrm{e}^{-\alpha x},$$

where C and α are constants. Apply continuity boundary conditions at $x = +L/2$ to find a relationship between k, L and α that does not include the constants A and C.

Exercise 8.3 A one-dimensional infinite well is described by the potential energy function

$$V(x) = \begin{cases} 0 & \text{for } -L/2 < x < 0 \\ V_0 & \text{for } 0 < x < L/2 \\ \infty & \text{elsewhere,} \end{cases}$$

where V_0 is a positive constant. An energy eigenfunction for a particle inside this well takes the form

$$\psi(x) = \begin{cases} A\cos(k_1 x) + B\sin(k_1 x) & \text{for } -L/2 < x < 0 \\ C\cos(k_2 x) + D\sin(k_2 x) & \text{for } 0 < x < L/2 \\ 0 & \text{elsewhere,} \end{cases}$$

where A, B, C, D, k_1 and k_2 are constants.

Use the time-independent Schrödinger equation to find a relationship between k_1, k_2, V_0 and the mass m of the particle.

Exercise 8.4 Consider again the situation described in Exercise 8.3. Use appropriate boundary conditions at $x = -L/2$, $x = L/2$ and $x = 0$ to find a relationship between k_1, k_2 and L that does not involve the constants A, B, C or D

Topic 9 — The overlap rule

Exercise 9.1 (a) State the overlap rule for energy measurements in a state described by the wave function $\Psi(x, t)$ in a system with discrete non-degenerate energy levels.

(b) Supposing that a system is described by a wave function that is an even function of x, use the overlap rule to show that there is no chance that any measurement of the system's energy will give a value that corresponds to an energy eigenfunction that is an odd function of x.

Exercise 9.2 A system has energy eigenfunctions $\psi_1(x)$, $\psi_2(x)$, ..., with corresponding energy eigenvalues E_1, E_2, ... If the system is in a state described by the energy eigenfunction $\psi_1(x)$, what is the probability of getting the value $E_2 \neq E_1$ in an energy measurement? Use your answer to show that the overlap rule implies that the eigenfunctions $\psi_1(x)$ and $\psi_2(x)$ must be orthogonal.

Exercise 9.3 A particle of mass m is in a one-dimensional infinite square well with walls at $x = -L/2$ and $x = +L/2$. At $t = 0$, the particle is described by the normalized wave function

$$\Psi(x,0) = \begin{cases} \frac{1}{\sqrt{w}} & \text{for } -w/2 \le x \le w/2 \\ 0 & \text{elsewhere,} \end{cases}$$

where $0 < w \le L$. If the energy of the particle is measured at time $t = 0$, what is the probability that the ground-state energy eigenvalue $E_1 = \pi^2\hbar^2/2mL^2$ will be obtained?

Topic 10 — The coefficient rule

Exercise 10.1 At time $t = 0$, the state of a particle is represented by a wave function of the form

$$\Psi(x,0) = \frac{1}{2}\psi_1(x) + \alpha\psi_2(x),$$

where $\psi_1(x)$ and $\psi_2(x)$ are normalized energy eigenfunctions corresponding to different energy eigenvalues E_1 and E_2. Find a possible value of α that ensures that $\Psi(x,0)$ is correctly normalized. Would the state be changed by changing the phase of α?

Exercise 10.2 At time $t = 0$, the wave function describing the state of a system takes the form

$$\Psi(x,0) = 2N\psi_1(x) - \sqrt{5}N\psi_2(x),$$

where $\psi_1(x)$ and $\psi_2(x)$ are normalized energy eigenfunctions with energy eigenvalues $E_1 = \varepsilon$ and $E_2 = 2\varepsilon$ respectively. Find a suitable value for the normalization constant N, and determine the expectation value of the energy at time $t = 0$.

Exercise 10.3 A system is in a state described by the wave function

$$\Psi(x,t) = A\big(\psi_1(x)\mathrm{e}^{-\mathrm{i}E_1t/\hbar} - \mathrm{i}\psi_2(x)\mathrm{e}^{-\mathrm{i}E_2t/\hbar}\big),$$

where $\psi_1(x)$ and $\psi_2(x)$ are orthonormal energy eigenfunctions corresponding to the eigenvalues E_1 and E_2 respectively. Find a suitable value for the normalization constant A and determine the expectation value of the energy at any time t.

Exercise 10.4 Three normalized stationary-state wave functions $\psi_1(x)\,\mathrm{e}^{-\mathrm{i}E_1t/\hbar}$, $\psi_2(x)\,\mathrm{e}^{-\mathrm{i}E_2t/\hbar}$ and $\psi_3(x)\,\mathrm{e}^{-\mathrm{i}E_3t/\hbar}$, corresponding to energies E_1, E_2 and E_3, are added with coefficients a_1, a_2 and a_3 to produce the wave function

$$\Psi(x,t) = a_1\,\psi_1(x)\,\mathrm{e}^{-\mathrm{i}E_1t/\hbar} + a_2\,\psi_2(x)\,\mathrm{e}^{-\mathrm{i}E_2t/\hbar} + a_3\,\psi_3(x)\,\mathrm{e}^{-\mathrm{i}E_3t/\hbar}.$$

(a) Write down the condition that must be satisfied by a_1, a_2 and a_3 in order for the wave function $\Psi(x,t)$ to be normalized.

(b) If the coefficients a_1, a_2 and a_3 are all multiplied by -1, will this make any difference to the expectation value of the position x?

(c) If a_1 alone is multiplied by -1, will this, in general, make any difference to the expectation value of the position x?

(d) If a_1 alone is multiplied by -1, will this, in general, make any difference to the expectation value of the energy, E?

Topic 11 — The sandwich integral rule

Exercise 11.1 (a) State the sandwich integral rule for the expectation value of an observable A in a system of one particle in one dimension.

(b) At $t = 0$, a particle is in a state described by the wave function

$$\Psi(x,0) = A\mathrm{e}^{-\alpha x^2},$$

where α and A are constants and $\alpha > 0$. Find the expectation values of x and p_x in this state.

Exercise 11.2 The normalized energy eigenfunctions of a particle in a one-dimensional infinite square well with walls at $x = 0$ and $x = L$ are

$$\psi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}} \sin\left(\dfrac{n\pi x}{L}\right) & \text{for } 0 \leq x \leq L \\ 0 & \text{elsewhere,} \end{cases}$$

for $n = 1,\ 2,\ \ldots$.

Calculate $\langle x^2 \rangle$ in the state with quantum number n.

You may use the standard integral

$$\int_0^{n\pi} u^2 \sin^2 u \, du = \frac{n\pi}{12}(2n^2\pi^2 - 3).$$

Exercise 11.3 Find the expectation value of the observable p_x^2 in the state described by the normalized wave function

$$\Psi(x,0) = \left(\frac{1}{\sqrt{\pi}a}\right)^{1/2} e^{-x^2/2a^2}.$$

You may use the fact that

$$\frac{d^2}{dx^2}\left(e^{-x^2/2a^2}\right) = \frac{1}{a^2}\left(\frac{x^2}{a^2} - 1\right) e^{-x^2/2a^2}$$

together with the standard integrals

$$\int_{-\infty}^{\infty} e^{-u^2} \, du = \sqrt{\pi} \quad \text{and} \quad \int_{-\infty}^{\infty} u^2 e^{-u^2} \, du = \frac{\sqrt{\pi}}{2}.$$

Exercise 11.4 Find the expectation value of the observable $e^{-\lambda^2 x^2}$, where λ is a real constant in the state described by the normalized wave function

$$\Psi(x,0) = \left(\frac{1}{\sqrt{\pi}a}\right)^{1/2} e^{-x^2/2a^2}.$$

You may use the standard integral

$$\int_{-\infty}^{\infty} e^{-\alpha u^2} \, du = \sqrt{\frac{\pi}{\alpha}},$$

for any positive constant, α.

Topic 12 — Uncertainties and the uncertainty principle

Exercise 12.1 At $t = 0$, a particle is in a state described by the normalized wave function

$$\Psi(x,0) = \frac{\sqrt{3}}{2}\psi_1(x) + \frac{i}{2}\psi_2(x),$$

where $\psi_1(x)$ is a normalized energy eigenfunction with eigenvalue $E_1 = \varepsilon$ and $\psi_2(x)$ is a normalized energy eigenfunction with eigenvalue $E_2 = 2\varepsilon$. Find the expectation value and uncertainty of the energy in this state.

Exercise 12.2 A particle is in a state characterized by the expectation values $\langle x \rangle = 1.0\,\text{nm}$ and $\langle x^2 \rangle = 2.0\,\text{nm}^2$.

(a) What is the uncertainty in x in this state?

(b) According to the Heisenberg uncertainty principle, what are the minimum values of the uncertainties in p_x and p_y that could be consistent with this uncertainty in x?

Topic 13 — Harmonic oscillators

Exercise 13.1 Verify that the function $\psi(x) = \mathrm{e}^{-\alpha x^2}$, where α is a positive constant, is a solution of the time-independent Schrödinger equation for a harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \tfrac{1}{2}Cx^2\psi(x) = E\psi(x),$$

provided that α has an appropriate value, which you are asked to find. Also find the corresponding energy eigenvalue, E.

Exercise 13.2 A harmonic oscillator has a zero-point energy of $1.5\,\mathrm{eV}$. What is the wavelength of the light emitted when this oscillator makes a radiative transition from a state with quantum number $n = 5$ to a state of lower energy?

Exercise 13.3 Use raising and lowering operators to show that

$$\langle \widehat{\mathrm{x}}\,\widehat{\mathrm{p}}_x \rangle = \frac{\mathrm{i}\hbar}{2}$$

in any energy eigenstate of a harmonic oscillator.

Exercise 13.4 (a) If $\widehat{\mathrm{A}}$ and $\widehat{\mathrm{A}}^\dagger$ are lowering and raising operators for a harmonic oscillator, show that

$$I = \int_{-\infty}^{\infty} \psi_n^*(x)\left[(\widehat{\mathrm{A}} + \widehat{\mathrm{A}}^\dagger)^2 + (\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger)^2\right]\psi_n(x)\,\mathrm{d}x = 0,$$

where $\psi_n(x)$ is an energy eigenfunction of the harmonic oscillator.

(b) Hence use the formulae

$$\widehat{\mathrm{x}} = \frac{a}{\sqrt{2}}(\widehat{\mathrm{A}} + \widehat{\mathrm{A}}^\dagger) \quad \text{and} \quad \widehat{\mathrm{p}}_x = \frac{-\mathrm{i}\hbar}{\sqrt{2}a}(\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger)$$

to show that

$$\frac{\langle x^2 \rangle}{a^2} = \frac{a^2\langle p_x^2 \rangle}{\hbar^2}$$

in any energy eigenstate of the harmonic oscillator. Given that $a^4 = \hbar^2/mC$, where m is the mass of the oscillating particle and C is the force constant of the harmonic oscillator, what is the physical interpretation of this result?

Topic 14 — Bound-state wave packets

Exercise 14.1 At time $t = 0$, a wave packet describing the state of a particle in a harmonic potential energy well takes the form

$$\Psi(x, 0) = \frac{1}{\sqrt{2}}\left(\psi_1(x) + \mathrm{i}\psi_2(x)\right),$$

where $\psi_1(x)$ and $\psi_2(x)$ are normalized energy eigenfunctions of the harmonic oscillator with eigenvalues $\frac{3}{2}\hbar\omega_0$ and $\frac{5}{2}\hbar\omega_0$, respectively, and ω_0 is the classical angular frequency of the oscillator.

(a) Write down an expression for $\Psi(x, t)$ at any later time t, expressing your answer in terms of ω_0.

(b) Are there any times after $t = 0$ when $\Psi(x, t)$ is orthogonal to the initial wave packet, $\Psi(x, 0)$?

Exercise 14.2 (a) A wave packet describing the state of a particle in a harmonic potential energy well takes the form

$$\Psi(x, t) = \frac{1}{\sqrt{2}}\left(\psi_0(x)\,\mathrm{e}^{-\mathrm{i}E_0t/\hbar} + \psi_2(x)\,\mathrm{e}^{-\mathrm{i}E_2t/\hbar}\right),$$

where $\psi_0(x)$ and $\psi_2(x)$ are normalized energy eigenfunctions for the ground state and second-excited state of the oscillator, with energy eigenvalues $E_0 = \frac{1}{2}\hbar\omega_0$ and $E_2 = \frac{5}{2}\hbar\omega_0$, respectively, where ω_0 is the classical angular frequency. Show that the probability density for this wave packet oscillates with period π/ω_0.

(b) What is the relationship between $\Psi(x, t)$ and $\Psi(-x, t)$? Does the motion of the wave packet correspond to a to-and-fro classical oscillation?

Topic 15 — Free-particle wave packets

Exercise 15.1 At time $t = 0$, a one-dimensional wave packet for a free particle of mass m takes the form

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, \mathrm{e}^{\mathrm{i}kx}\, \mathrm{d}k.$$

Write down an expression for the wave packet at a later time, t, defining any quantities you introduce. What is the physical significance of the function $A(k)$ with respect to measurements of momentum?

Exercise 15.2 (a) At time $t = 0$, a one-dimensional wave packet for a free particle of mass m takes the form

$$\Psi(x,0) = \begin{cases} \frac{1}{\sqrt{L}}\, \mathrm{e}^{\mathrm{i}\alpha x} & \text{for } -L/2 \le x \le L/2 \\ 0 & \text{elsewhere,} \end{cases}$$

where α is a real constant. What is the momentum amplitude function for this wave packet?

(b) Assuming that $\alpha = 1/L$ and using the fact that

$$\int_0^1 \frac{\sin^2(u)}{u^2}\, \mathrm{d}u = 0.897,$$

calculate the probability that a momentum measurement taken on the wave packet at $t = 0$ will give a value between $-\hbar\alpha$ and $+\hbar\alpha$.

Exercise 15.3 (a) Explain why the following solution to the free-particle Schrödinger equation:

$$\Psi_{\text{dB}}(x,t) = A\mathrm{e}^{\mathrm{i}(kx - E_k t/\hbar)},$$

where A is a constant and $E_k = \hbar^2 k^2/2m$, is not entirely satisfactory for representing the state of a free particle in one dimension.

(b) Consider the following expression for a normalized free particle wave packet:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, \mathrm{e}^{\mathrm{i}(kx - E_k t/\hbar)} \mathrm{d}k.$$

Write an expression involving $A(k)$ that is equal to the probability that a momentum measurement made on a particle described by $\Psi(x,t)$ will yield a value between $\hbar k_1$ and $\hbar k_2$.

What condition must $A(k)$ satisfy in order for $\Psi_{\text{dB}}(x,t)$ to be normalized?

Topic 16 — Ehrenfest's theorem

Exercise 16.1 State Ehrenfest's theorem for $\langle x \rangle$ and $\langle p_x \rangle$ for a particle of mass m subject to a potential energy function $V(x)$. Show that, if $V(x) = mgx$, where g is a constant, then Ehrenfest's theorem gives

$$\frac{\mathrm{d}^2 \langle x \rangle}{\mathrm{d}t^2} = -g.$$

Topic 17 — Scattering and tunnelling

Exercise 17.1 A mono-energetic beam of particles, travelling in the x-direction is incident on a step located at $x = 0$. In Region 1 ($x \le 0$) the beam is described by the energy eigenfunction

$$\psi_1(x) = A\mathrm{e}^{\mathrm{i}k_1 x} + B\mathrm{e}^{-\mathrm{i}k_1 x}$$

where A and B are constants. In Region 2 ($x \ge 0$) the beam is described by the energy eigenfunction

$$\psi_2(x) = C\mathrm{e}^{\mathrm{i}k_2 x},$$

where C is a constant. Use appropriate boundary conditions at $x = 0$ to relate A and B to C and hence determine the ratio B/A in terms of the wave numbers k_1 and k_2.

Exercise 17.2 A mono-energetic beam of particles, travelling in the x-direction is incident on a step located at $x = 0$. In Region 1 ($x \leq 0$) the beam is described by the energy eigenfunction

$$\psi_1(x) = A\mathrm{e}^{\mathrm{i}k_1x} + B\mathrm{e}^{-\mathrm{i}k_1x},$$

where A and B are constants and k_1 is real. In Region 2 ($x \geq 0$) the beam is described by the energy eigenfunction

$$\psi_2(x) = C\mathrm{e}^{-\alpha x},$$

where C is a constant and α is real. Use appropriate boundary conditions at $x = 0$ to relate A and B to C and hence show that $|B/A|^2 = 1$.

Exercise 17.3 Find the probability current associated with the free-particle energy eigenfunction $\psi(x) = A\mathrm{e}^{\mathrm{i}kx}$, where A is a constant.

Solutions

Topic 1 — de Broglie waves

Solution 1.1 (a) A one-dimensional de Broglie wave, travelling in the positive x-direction, takes the form

$$\Psi_{\text{dB}}(x,t) = \mathrm{e}^{\mathrm{i}(kx-\omega t)},$$

where k is the wave number and ω is the angular frequency of the wave. For the de Broglie wave given in the question we have

$$k = A = 3.20 \times 10^{10}\,\text{m}^{-1} \quad \text{and} \quad \omega = B = 7.44 \times 10^{14}\,\text{s}^{-1}.$$

The wave number and angular frequency are related to the wavelength λ and period T by $k = 2\pi/\lambda$ and $\omega = 2\pi/T$, so

$$\lambda = \frac{2\pi}{k} = \frac{2\pi}{3.20 \times 10^{10}\,\text{m}^{-1}} = 1.96 \times 10^{-10}\,\text{m}$$

and

$$T = \frac{2\pi}{\omega} = \frac{2\pi}{7.44 \times 10^{14}\,\text{s}^{-1}} = 8.45 \times 10^{-15}\,\text{s}.$$

(b) The momentum magnitude is

$$p = \hbar k = 1.06 \times 10^{-34}\,\text{J s} \times 3.20 \times 10^{10}\,\text{m}^{-1} = 3.39 \times 10^{-24}\,\text{kg m s}^{-1}.$$

The energy of the particle is

$$E = \hbar\omega = 1.06 \times 10^{-34}\,\text{J s} \times 7.44 \times 10^{14}\,\text{s}^{-1} = 7.89 \times 10^{-20}\,\text{J},$$

and, since the particle is free with zero potential energy everywhere, this is equal to the kinetic energy, E_{kin}.

Finally, the kinetic energy and momentum magnitude of the particle are related by $E_{\text{kin}} = p^2/2m$, so the mass of the particle is

$$m = \frac{p^2}{2E_{\text{kin}}} = \frac{(3.39 \times 10^{-24}\,\text{kg m s}^{-1})^2}{2 \times 7.89 \times 10^{-20}\,\text{J}} = 7.28 \times 10^{-29}\,\text{kg}.$$

Comments (1) The units of λ, T and p are all correct. For mass we have $\text{J} = \text{kg m}^2\,\text{s}^{-2}$, so $(\text{kg m s}^{-1})^2/\text{J} = \text{kg}$, as required.

(2) You may know from elsewhere in physics that the *phase speed* of any wave is given by $v_{\text{wave}} = f\lambda = \omega/k$. Please note, however, that the phase speed of a de Broglie wave is not equal to the speed of the free particle it describes, which is given by p/m. According to the last equation in the solution, the speed of the particle is $p/m = 2E_{\text{kin}}/p = 2\omega/k$, which is twice the phase speed of the wave!

Solution 1.2 We have

$$\begin{aligned}
\widehat{\mathrm{p}}_x \Psi_{\text{dB}}(x,t) &= -\mathrm{i}\hbar \frac{\partial}{\partial x} \mathrm{e}^{2\pi \mathrm{i}(x/\lambda - t/T)} \\
&= -\mathrm{i}\hbar\, \frac{2\pi\mathrm{i}}{\lambda}\, \mathrm{e}^{2\pi \mathrm{i}(x/\lambda - t/T)} \\
&= \frac{2\pi\hbar}{\lambda} \mathrm{e}^{2\pi \mathrm{i}(x/\lambda - t/T)},
\end{aligned}$$

so $\Psi_{\text{dB}}(x,t)$ is an eigenfunction of $\widehat{\mathrm{p}}_x$, with eigenvalue $2\pi\hbar/\lambda = h/\lambda$, where h is Planck's constant. The positive constant λ is the wavelength of the wave (i.e. the distance between points that have the same phase at a given instant). So this result is consistent with the de Broglie relation, $\lambda = h/p$.

Comment To check whether any function is an eigenfunction of a given operator, apply the operator to the function and see whether you get the same function back, multiplied by a constant (the eigenvalue).

Topic 2 — Operators

Solution 2.1 $\widehat{\mathrm{O}}_1$ is linear because, if λ and μ are arbitrary constants,

$$\begin{aligned}\widehat{\mathrm{O}}_1(\lambda f(x)+\mu g(x)) &\equiv x^2(\lambda f(x)+\mu g(x))\\ &= \lambda x^2 f(x)+\mu x^2 g(x)\\ &\equiv \lambda\big(\widehat{\mathrm{O}}_1 f(x)\big)+\mu\big(\widehat{\mathrm{O}}_1 g(x)\big).\end{aligned}$$

$\widehat{\mathrm{O}}_2$ is *not* linear because, if λ and μ are arbitrary constants,

$$\begin{aligned}\widehat{\mathrm{O}}_2(\lambda f(x)+\mu g(x)) &\equiv [\lambda f(x)+\mu g(x)]^2\\ &= \lambda^2 f^2(x)+\mu^2 g^2(x)+2\lambda\mu\, f(x)\, g(x)\\ &= \lambda^2\big(\widehat{\mathrm{O}}_2 f(x)\big)+\mu^2\big(\widehat{\mathrm{O}}_2 g(x)\big)+2\lambda\mu\, f(x)\, g(x)\\ &\neq \lambda\big(\widehat{\mathrm{O}}_2 f(x)\big)+\mu\big(\widehat{\mathrm{O}}_2 g(x)\big)\quad\text{(in general).}\end{aligned}$$

$\widehat{\mathrm{O}}_3$ is linear because, if λ and μ are arbitrary constants,

$$\begin{aligned}\widehat{\mathrm{O}}_3(\lambda f(x)+\mu g(x)) &\equiv \lambda f(x+a)+\mu g(x+a)\\ &\equiv \lambda\big(\widehat{\mathrm{O}}_3 f(x)\big)+\mu\big(\widehat{\mathrm{O}}_3 g(x)\big).\end{aligned}$$

Comment To check whether a given operator is linear, we always start by applying the operator to a general linear combination of functions $\lambda f+\mu g$ and then try to rearrange the result.

Solution 2.2 We have

$$\begin{aligned}\widehat{\mathrm{O}}_1\widehat{\mathrm{O}}_2 g(x) &= \widehat{\mathrm{O}}_1\big(\widehat{\mathrm{O}}_2 g(x)\big)\\ &= \frac{\mathrm{d}}{\mathrm{d}x}\big(x^2 g(x)\big)\\ &= 2xg(x)+x^2\frac{\mathrm{d}g(x)}{\mathrm{d}x},\end{aligned}$$

while

$$\widehat{\mathrm{O}}_2\widehat{\mathrm{O}}_1 g(x) = \widehat{\mathrm{O}}_2\big(\widehat{\mathrm{O}}_1 g(x)\big) = x^2\frac{\mathrm{d}g(x)}{\mathrm{d}x}.$$

Subtracting these two results we obtain

$$\big(\widehat{\mathrm{O}}_1\widehat{\mathrm{O}}_2-\widehat{\mathrm{O}}_2\widehat{\mathrm{O}}_1\big)g(x) = 2xg(x).$$

Comments (1) When simplifying $\widehat{\mathrm{O}}_1\widehat{\mathrm{O}}_2\,(g(x))$, note that the derivative operator $\widehat{\mathrm{O}}_1=\mathrm{d}/\mathrm{d}x$ acts on $x^2 g(x)$, which must be differentiated using the product rule. This gives a different result from $\widehat{\mathrm{O}}_2\widehat{\mathrm{O}}_1 g(x)\equiv x^2\mathrm{d}g/\mathrm{d}x$, so the order of the operators matters (they do not commute).

(2) Since the final equation is valid for any function $g(x)$, we can also express it as a relation between operators:

$$\widehat{\mathrm{O}}_1\widehat{\mathrm{O}}_2-\widehat{\mathrm{O}}_2\widehat{\mathrm{O}}_1 = 2x,$$

where the expression on the left-hand side is called the *commutator* of the operators $\widehat{\mathrm{O}}_1$ and $\widehat{\mathrm{O}}_2$.

Topic 3 — Schrödinger's equation

Solution 3.1 The Hamiltonian function is

$$H = \frac{p_{x,1}^2}{2m_1} + \frac{p_{x,2}^2}{2m_2} + \tfrac{1}{2}C(x_1 - x_2)^2,$$

where $p_{x,1}$ and $p_{x,2}$ are the momenta of the two particles.

Since $\widehat{\mathrm{p}} = -\mathrm{i}\hbar\partial/\partial x$ and $\widehat{\mathrm{p}}^2 = -\hbar^2\partial^2/\partial x^2$, the corresponding Hamiltonian operator is

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + \tfrac{1}{2}C(x_1 - x_2)^2.$$

Schrödinger's equation then takes the form

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x_1, x_2, t) = -\frac{\hbar^2}{2m_1}\frac{\partial^2\Psi(x_1, x_2, t)}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2\Psi(x_1, x_2, t)}{\partial x_2^2} + \tfrac{1}{2}C(x_1 - x_2)^2\Psi(x_1, x_2, t).$$

Comment We introduce separate position variables (x_1 and x_2) and momentum variables ($p_{x,1}$ and $p_{x,2}$) for the two particles. The wave function $\Psi(x_1, x_2, t)$ of the two-particle system depends on both x_1 and x_2, as well as on time, t.

Solution 3.2 The Hamiltonian function is

$$H = \frac{p_{x,1}^2}{2m_1} + \frac{p_{x,2}^2}{2m_2} + \tfrac{1}{2}Cx_1^2 + \tfrac{1}{2}Cx_2^2.$$

The corresponding Hamiltonian operator is

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + \tfrac{1}{2}Cx_1^2 + \tfrac{1}{2}Cx_2^2.$$

Schrödinger's equation then takes the form

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x_1, x_2, t) = -\frac{\hbar^2}{2m_1}\frac{\partial^2\Psi(x_1, x_2, t)}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2\Psi(x_1, x_2, t)}{\partial x_2^2} + \left(\tfrac{1}{2}Cx_1^2 + \tfrac{1}{2}Cx_2^2\right)\Psi(x_1, x_2, t).$$

Comment In Exercise 3.1 the particles interacted directly with one another via a potential energy function that depends on $(x_1 - x_2)^2$, the square of the separation of the particles. The situation described in this question is different because the two particles do not interact with one another, but each particle is subject to a potential energy function (due to an external agency) which depends on the square of the separation of the particle from the origin ($\tfrac{1}{2}Cx_1^2$ for particle 1 and $\tfrac{1}{2}Cx_2^2$ for particle 2).

Solution 3.3 (a) For a free particle of mass m in one dimension, Schrödinger's equation takes the form

$$\mathrm{i}\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}.$$

If $\Psi_1(x,t)$ and $\Psi_2(x,t)$ are both solutions of this form of Schrödinger's equation, and c_1 and c_2 are any constants, we have

$$\begin{aligned}
&\left(\mathrm{i}\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Big(c_1\Psi_1(x,t) + c_2\Psi_2(x,t)\Big) \\
&= c_1\left(\mathrm{i}\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi_1(x,t) + c_2\left(\mathrm{i}\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi_2(x,t) \\
&= c_1 \times 0 + c_2 \times 0 = 0,
\end{aligned}$$

because $\Psi_1(x,t)$ and $\Psi_2(x,t)$ separately satisfy the free-particle form of Schrödinger's equation. So any linear combination of the form $c_1\Psi_1(x,t) + c_2\Psi_2(x,t)$ is also a solution of the free-particle form of Schrödinger's equation, consistent with the principle of superposition.

(b) If the solution of Schrödinger's equation corresponding to passage through one slit is Ψ_1 and the solution corresponding to passage through the other slit is Ψ_2, the principle of superposition tells us that a normalized combination $A(\Psi_1 + \Psi_2)$ is also a solution of Schrödinger's equation. The probability density for electrons arriving on the screen is given by $|\Psi_1 + \Psi_2|^2$, and this displays peaks where Ψ_1 and Ψ_2 interfere constructively and troughs where Ψ_1 and Ψ_2 interfere destructively.

Comments (1) An equation is linear if it can be written in the form $\widehat{\mathrm{L}}f(x)$, where $\widehat{\mathrm{L}}$ is a linear operator. That is why we moved the right-hand side of Schrödinger's equation to the left, and then used the method of Exercise 2.1.

(2) The question refers to Schrödinger's equation which should never be confused with the time-independent Schrödinger equation. Both equations depend on the system under study, but they have very different roles: Schrödinger's equation tells us how any wave function for the system evolves in time, while the time-independent Schrödinger equation tells us about the possible energies of the system and the corresponding energy eigenfunctions.

Topic 4 — Separation of variables

Solution 4.1 (a) Substituting $\Psi(x,t) = \psi(x)T(t)$ in Schrödinger's equation gives

$$\psi(x)\mathrm{i}\hbar\frac{\mathrm{d}T}{\mathrm{d}t} = -T(t)\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi(x)T(t).$$

Dividing through by $\psi(x)T(t)$ and rearranging then gives

$$\frac{1}{T(t)}\mathrm{i}\hbar\frac{\mathrm{d}T}{\mathrm{d}t} = -\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x).$$

The two sides of this equation depend on different variables, so they must both be equal to the same constant, E. We therefore get two equations:

$$-\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x) = E$$

$$\frac{1}{T(t)}\mathrm{i}\hbar\frac{\mathrm{d}T}{\mathrm{d}t} = E,$$

which can be written as

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -(\mathrm{i}E/\hbar)T(t).$$

The general solution of the second equation is $T(t) = C\mathrm{e}^{-\mathrm{i}Et/\hbar}$, where C is an arbitrary constant. (This constant is generally chosen to be equal to 1; there is no loss in generality in doing this because the arbitrary constants accompanying $T(t)$ and $\psi(x)$ are multiplied together in the product function $\psi(x)T(t)$.)

(b) Not all solutions of Schrödinger's equation can be written in the form of a product of a function of position and a function of time. Because Schrödinger's equation is linear, any linear combination of solutions is also a solution, so a solution of the form

$$\Psi(x,t) = \sum_i a_i\,\psi_i(x)\,\mathrm{e}^{-\mathrm{i}E_it/\hbar}$$

will satisfy Schrödinger's equation, although it is not itself in a separated (i.e. stationary state) form.

Comments (1) The natural way to start this question is to substitute the given form of wave function $\Psi(x,t) = \psi(x)T(t)$ into Schrödinger's equation. The key step is then to rearrange the equation so that one side involves only functions of x and the other side involves only functions of t. This is achieved by dividing by $\psi(x)T(t)$.

(2) Note that the first line of the solution uses ordinary derivatives rather than partial derivatives. This is appropriate because $\psi(x)$ and $T(t)$ are both functions of a single variable, so $\partial\psi/\partial x$ and $\partial T/\partial t$ can only mean $\mathrm{d}\psi/\mathrm{d}x$ and $\mathrm{d}T/\mathrm{d}t$, respectively.

Solution 4.2 Substituting $\psi(x, y, z) = X(x)Y(y)Z(z)$ in the time-independent Schrödinger equation gives

$$-\frac{\hbar^2}{2m}\left(Y(y)Z(z)\frac{\mathrm{d}^2X}{\mathrm{d}x^2} + X(x)Z(z)\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} + X(x)Y(y)\frac{\mathrm{d}^2Z}{\mathrm{d}z^2}\right) = EX(x)Y(y)Z(z).$$

Dividing both sides by $X(x)Y(y)Z(z)$ then gives

$$-\frac{\hbar^2}{2m}\left(\frac{1}{X(x)}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} + \frac{1}{Y(y)}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} + \frac{1}{Z(z)}\frac{\mathrm{d}^2Z}{\mathrm{d}z^2}\right) = E.$$

The three terms in the round brackets on the left-hand side are functions of different variables. The only way the left-hand side of the equation can be equal to the constant on the right-hand side is for each of these terms to be equal to a constant. We therefore have

$$\frac{1}{X(x)}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} = C_x$$

$$\frac{1}{Y(y)}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} = C_y$$

$$\frac{1}{Z(z)}\frac{\mathrm{d}^2Z}{\mathrm{d}z^2} = C_z.$$

Substituting these equations back into the unseparated equation, we see that

$$-\frac{\hbar^2}{2m}(C_x + C_y + C_z) = E.$$

Comments (1) The method of separation of variables works for partial differential equations involving many variables, just as well as for those involving two variables. It can be applied step-by-step, splitting off one variable at a time, but here we have used it more efficiently relying on the fact that if a sum like $f(x) + g(y) + h(z)$ is equal to a constant for all values of x, y and z, it follows that $f(x)$, $g(y)$ and $h(z)$ are each equal to constants.

(2) In the last line of the solution, it turns out that C_x is negative, and is normally written as $-k_x^2$, with similar notations for C_y and C_z. However, the proof of this fact requires consideration of the boundary conditions, and is not part of this question.

Topic 5 — Born's rule

Solution 5.1 (a) In one dimension, Born's rule states that the probability at time t of finding the particle in a small interval of width δx, centred on x, is $|\Psi(x,t)|^2\,\delta x$.

(b) The required probability is

$$\begin{aligned}\text{probability} &= |\Psi(x,t)|^2\,\delta x \\ &= \left(\sqrt{\frac{2}{L}}\sin(0.25\pi)\,\mathrm{e}^{-\mathrm{i}Et/\hbar}\right)^*\left(\sqrt{\frac{2}{L}}\sin(0.25\pi)\,\mathrm{e}^{-\mathrm{i}Et/\hbar}\right) \times 0.002L \\ &= \frac{2}{L}\sin^2(0.25\pi)\,\mathrm{e}^{+\mathrm{i}Et/\hbar}\mathrm{e}^{-\mathrm{i}Et/\hbar} \times 0.002L \\ &= \frac{2}{L} \times \frac{1}{2} \times 0.002L = 0.002.\end{aligned}$$

This probability does not depend on time because the time-dependent phase factor $\mathrm{e}^{-\mathrm{i}Et/\hbar}$ is removed by taking the modulus of the wave function.

Comments (1) The wording of this exercise includes the words 'small interval'. This is effectively an invitation to use Born's rule without integrating over an extended range: we are assuming that the wave function is practically constant over the small interval from $0.249L$ to $0.251L$, and that the appropriate value to use throughout this region is $\Psi(0.25, t)$.

(2) The probability works out to be a real number between 0 and 1, as it must.

Solution 5.2 The probability of finding the particle between $x = 0$ and $x = L/5$ at $t = 0$ is

$$\text{probability} = \frac{2}{L}\int_0^{L/5} \sin^2\left(\frac{5\pi x}{L}\right) \mathrm{d}x.$$

We change the variable of integration to $u = 5\pi x/L$. Then $x = 0$ corresponds to $u = 0$ and $x = L/5$ corresponds to $u = \pi$. Also, $x = (L/5\pi)u$ and $\mathrm{d}x = (L/5\pi)\,\mathrm{d}u$, so

$$\begin{aligned}\text{probability} &= \frac{2}{L}\left(\frac{L}{5\pi}\right)\int_0^{\pi} \sin^2 u \,\mathrm{d}u \\ &= \frac{2}{L}\frac{L}{5\pi}\frac{\pi}{2} = \frac{1}{5}.\end{aligned}$$

Comments (1) In this exercise, the given interval cannot be treated as small in the context of using Born's rule (no matter what the value of L). This is because the wave function varies significantly across the interval. We cannot use Born's rule directly, but must integrate the probability density $|\Psi(x,0)|^2$ over the interval, from $x = 0$ to $x = L/5$.

(2) This question could also be answered by drawing a sketch of $|\Psi(x,0)|^2$ between $x = 0$ and $x = L$, noting that it consists of 5 peaks, each of the same area, and remembering that the area under the whole graph must be equal to 1.

Solution 5.3 (a) For $x > L/2$, the probability density for finding the particle at position x is

$$|\psi_1(x)|^2 = \left(C\mathrm{e}^{-\alpha x}\right)^* C\mathrm{e}^{-\alpha x} = |C|^2\mathrm{e}^{-2\alpha x}.$$

Hence the probability of finding the particle anywhere with $x > L/2$ is

$$P_{x>L/2} = \int_{L/2}^{\infty} |C|^2\mathrm{e}^{-2\alpha x}\,\mathrm{d}x = |C|^2\left[\frac{\mathrm{e}^{-2\alpha x}}{-2\alpha}\right]_{x=L/2}^{x=\infty} = |C|^2\frac{\mathrm{e}^{-\alpha L}}{2\alpha}.$$

For $x < -L/2$, the probability density for finding the particle at position x is

$$|\psi_1(x)|^2 = \left(C\mathrm{e}^{\alpha x}\right)^* C\mathrm{e}^{\alpha x} = |C|^2\mathrm{e}^{2\alpha x}.$$

Hence the probability of finding the particle anywhere with $x < -L/2$ is

$$P_{x<-L/2} = \int_{-\infty}^{-L/2} |C|^2\mathrm{e}^{2\alpha x}\,\mathrm{d}x = |C|^2\left[\frac{\mathrm{e}^{2\alpha x}}{2\alpha}\right]_{x=-\infty}^{x=-L/2} = |C|^2\frac{\mathrm{e}^{-\alpha L}}{2\alpha}.$$

The total probability of finding the particle somewhere outside the well is therefore

$$P_{\text{out}} = P_{x>L/2} + P_{x<-L/2} = \frac{|C|^2}{\alpha}\mathrm{e}^{-\alpha L}.$$

(b) The particle must be somewhere, so the probability of finding it to be somewhere *inside* the well is

$$P_{\text{in}} = 1 - \frac{|C|^2}{\alpha}\mathrm{e}^{-\alpha L}.$$

Comments (1) The region outside the well consists of two subregions: $-\infty < x < -L/2$ and $L/2 < x < \infty$. You need to include both of these to find the probability of detecting the particle outside the well.

(2) Rather than evaluating the integral from $-\infty$ to $-L/2$ directly, you could change the variable in this integral from x to $u = -x$; this would give an integral of the same form as that for the region from $L/2 < x < \infty$, so the contributions from the two subregions are the same.

(3) We have used the ground-state energy eigenfunction (rather than the corresponding stationary-state wave function) to find the probability because we know that the time-dependent phase factors in the stationary-state wave function Ψ and its complex conjugate Ψ^* cancel out in the product $\Psi^*\Psi$, leaving only a time-independent probability density (see Exercise 5.1 for example). The eigenfunction is equal to the stationary-state wave function at $t = 0$.

Solution 5.4 The particle is most likely to be found at the point where $|\Psi(x,0)|^2$ has its maximum value. We have

$$|\Psi(x,0)|^2 = |A|^2 x^2 \mathrm{e}^{-2x^2/a^2}.$$

The stationary values of this function are found by setting

$$\begin{aligned}
0 &= \frac{\mathrm{d}}{\mathrm{d}x}\left(|A|^2 x^2 \mathrm{e}^{-2x^2/a^2}\right) \\
&= |A|^2\left(\frac{\mathrm{d}}{\mathrm{d}x}(x^2)\times \mathrm{e}^{-2x^2/a^2} + x^2 \times \frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{-2x^2/a^2}\right)\right) \\
&= |A|^2\left(2x\mathrm{e}^{-2x^2/a^2} - \frac{4x^3}{a^2}\mathrm{e}^{-2x^2/a^2}\right) \\
&= 2x|A|^2\left(1-\frac{2x^2}{a^2}\right)\mathrm{e}^{-2x^2/a^2}.
\end{aligned}$$

This equation has solutions at $x = 0$ and $x = \pm a/\sqrt{2}$.

A rough sketch of the function shows that $x = 0$ corresponds to a minimum, and $x = \pm a/\sqrt{2}$ correspond to maxima, so the particle is most likely to be found at $x = \pm a/\sqrt{2}$.

Comment Some care is needed in doing the differentiation. The probability density involves a product of x^2 and e^{-2x^2/a^2}, which is differentiated using the product rule. The term e^{-2x^2/a^2} must be differentiated using the chain rule: we differentiate the exponential function (this gives the same function back again) and also multiply by the derivative of its contents:

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-2x^2/a^2} = \mathrm{e}^{-2x^2/a^2} \times \frac{\mathrm{d}}{\mathrm{d}x}(-2x^2/a^2) = -\frac{4x}{a^2}\mathrm{e}^{-2x^2/a^2}.$$

Solution 5.5 (a) In one dimension, Born's rule states that the probability of finding the particle in a small interval of width δx, centred on x, is $|\Psi(x,t)|^2\,\delta x$. Probabilities are dimensionless pure numbers, so $|\Psi(x,t)|^2$ must have the dimensions of length^{-1}. Hence $\Psi(x,t)$ has the dimensions of length$^{-1/2}$, and its SI units are $\mathrm{m}^{-1/2}$.

(b) (i) $f(x) = \mathrm{e}^{-\pi x^2/2a^2}$ is unsuitable because it is dimensionless (it would have to be multiplied by a suitable factor with dimensions of length$^{-1/2}$ in order to acquire the right dimensions.

(ii) $g(x) = (\sqrt{\pi/a})\,\mathrm{e}^{-x^2/2a^2}$ is appropriate on dimensional grounds because it has the dimensions of length$^{-1/2}$.

(iii) $h(x) = (\sqrt{\pi/a})\,\mathrm{e}^{-x^2/2}$ is unsuitable because the term $\mathrm{e}^{-x^2/2}$ has no consistent units. If it were expanded as a power series, it would give

$$1 + \left(\frac{-x^2}{2}\right) + \frac{1}{2!}\left(\frac{-x^2}{2}\right)^2 + \ldots.$$

Since x is a position coordinate with the dimensions of length, successive terms have different units; such terms cannot sensibly be added together. To make physical sense, arguments of functions like the exponential function must always be dimensionless.

Comments (1) It is worth remembering that any one-dimensional wave function has units of length$^{-1/2}$, and this can be a useful check. Note, however, that this is only true in one dimension. In three dimensions, wave functions have the dimensions of length$^{-3/2}$.

(2) Part (iii) relies on the convention used throughout physics where the position coordinate x is not a pure number, but is a number times a unit of length. This differs from some usages in maths, where the symbol x could perfectly well be a pure number (perhaps a ratio of two lengths).

Topic 6 — Normalization and phase

Solution 6.1 For the given wave function, the normalization condition is

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 \, \mathrm{d}x = |A|^2 \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/a^2} \, \mathrm{d}x.$$

Using the standard integral given in the question, this gives

$$1 = |A|^2 a\sqrt{\pi}.$$

A suitable choice for A is therefore

$$A = \left(\frac{1}{\sqrt{\pi}a}\right)^{1/2} = \left(\frac{1}{\pi a^2}\right)^{1/4}.$$

Any other value of the form

$$A = \left(\frac{1}{\pi a^2}\right)^{1/4} \mathrm{e}^{\mathrm{i}\alpha},$$

where α is real, could be chosen because any overall phase factor multiplying a wave function has no physical consequences.

Comment In spite of the freedom noted above, we would normally set $e^{\mathrm{i}\alpha} = 1$, giving the real positive value of A originally calculated. This has the advantage of simplifying any subsequent calculations made with the wave function.

Solution 6.2 We multiply the unnormalized eigenfunction $\phi(x)$ by a constant N, and then choose N to ensure normalization. Let

$$\psi(x) = N\phi(x).$$

Then we require that

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x \\ &= |N|^2 \int_{-\infty}^{\infty} |\phi(x)|^2 \, \mathrm{d}x \\ &= |N|^2 \int_0^L \sin^2\left(\frac{2\pi x}{L}\right) \mathrm{d}x. \end{aligned}$$

We change the variable of integration to $u = 2\pi x/L$. Then $x = 0$ corresponds to $u = 0$ and $x = L$ corresponds to $u = 2\pi$. Also, $x = (L/2\pi)u$ and $\mathrm{d}x = (L/2\pi)\,\mathrm{d}u$. So, using the standard integral given in the question,

$$\begin{aligned} 1 &= |N|^2 \frac{L}{2\pi} \int_0^{2\pi} \sin^2 u \, \mathrm{d}u \\ &= |N|^2 \frac{L}{2\pi} \times \pi \\ &= |N|^2 \frac{L}{2}. \end{aligned}$$

Hence a possible choice of N is $\sqrt{2/L}$ and the corresponding normalized eigenfunction is

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right).$$

Comments (1) Given an unnormalized wave function, with no adjustable constant, you are free to multiply it by an (as yet) undetermined constant N. Then you can use the same procedure as in Exercise 6.1 to find an appropriate value for that constant.

(2) It is often convenient to start a normalization calculation with the number 1 on the left-hand side of the equation, allowing a chain of equalities to flow in subsequent steps.

(3) Note how the limits of integration change from $x = \pm\infty$ to $x = 0$ and $x = L$ because the integrand vanishes outside this region.

Solution 6.3 Normalization requires that

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi(x,y,z)|^2 \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \\
&= |A|^2 \int_0^L\int_0^L\int_0^L \sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{2\pi y}{L}\right)\sin^2\left(\frac{3\pi z}{L}\right)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \\
&= |A|^2 \int_0^L \sin^2\left(\frac{\pi x}{L}\right)\mathrm{d}x \int_0^L \sin^2\left(\frac{2\pi y}{L}\right)\mathrm{d}y \int_0^L \sin^2\left(\frac{3\pi z}{L}\right)\mathrm{d}z.
\end{aligned}$$

For the integral over x, we change the variable of integration to $u = \pi x/L$, for the integral over y, we change the variable of integration to $v = 2\pi y/L$ and for the integral over z, we change the variable of integration to $w = 3\pi z/L$. Then

$$\begin{aligned}
1 &= |A|^2 \frac{L}{\pi}\frac{L}{2\pi}\frac{L}{3\pi}\int_0^{\pi}\sin^2 u\,\mathrm{d}u\int_0^{2\pi}\sin^2 v\,\mathrm{d}v\int_0^{3\pi}\sin^2 w\,\mathrm{d}w \\
&= |A|^2 \frac{L}{\pi}\frac{L}{2\pi}\frac{L}{3\pi}\times\frac{\pi}{2}\frac{2\pi}{2}\frac{3\pi}{2} \\
&= |A|^2\frac{L^3}{2^3},
\end{aligned}$$

so a suitable choice of A is $(2/L)^{3/2}$.

Comment Normalization in three dimensions involves a volume integral of the probability density. The present case uses Cartesian coordinates and, because of the product form of the wave function, the volume integral splits into a product of three separate integrals over x, y and z.

Solution 6.4 ψ_{C}, ψ_{E}, ψ_{F}, and ψ_{G} all represent the same state as ψ_{A} because they are equal to ψ_{A} times a phase factor. We have:

$$\begin{aligned}
\psi_{\mathrm{C}} &= \mathrm{i}\psi_{\mathrm{A}} = \mathrm{e}^{\mathrm{i}\pi/2}\psi_{\mathrm{A}} \\
\psi_{\mathrm{E}} &= -\mathrm{i}\psi_{\mathrm{A}} = \mathrm{e}^{-\mathrm{i}\pi/2}\psi_{\mathrm{A}} \\
\psi_{\mathrm{F}} &= \mathrm{e}^{\mathrm{i}\alpha}\psi_{\mathrm{A}} \\
\psi_{\mathrm{G}} &= \mathrm{e}^{\mathrm{i}(\alpha-\pi/2)}\psi_{\mathrm{A}}.
\end{aligned}$$

Comment To spot whether $\phi_{\mathrm{A}} = a_1\psi_1 + a_2\psi_2 + \ldots$ (with $a_1 \neq 0$) is a multiple of $\phi_{\mathrm{B}} = b_1\psi_1 + b_2\psi_2 + \ldots$, we can multiply ϕ_{A} by the factor b_1/a_1 that ensures its first term is the same as the first term in ϕ_{B}, and we can then check whether the remaining terms are also equal.

Topic 7 — Square wells

Solution 7.1 The energy levels for a particle of mass m in a three-dimensional cubic infinite square well with sides of length L are:

$$\frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2).$$

The ground state has quantum numbers $n_x = 1$, $n_y = 1$, $n_z = 1$, and energy

$$E_{\text{initial}} = \frac{3\pi^2\hbar^2}{2mL^2}.$$

When the sides of the box are shrunk to $L/2$, the ground-state energy becomes

$$E_{\text{final}} = \frac{3\pi^2\hbar^2}{2m(L/2)^2} = \frac{12\pi^2\hbar^2}{2mL^2}.$$

The change in energy is

$$\Delta E = E_{\text{final}} - E_{\text{initial}} = \frac{9\pi^2\hbar^2}{2mL^2}.$$

Comment The compression of a small quantum system can require considerable energy. This helps to explain why atoms display considerable rigidity in spite of being composed of very insubstantial particles (electrons) outside a tiny central nucleus.

Solution 7.2 The energy levels for a particle of mass m in a three-dimensional cubic infinite square well with sides of length L are:

$$\frac{\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2).$$

The states that have energy $3\hbar^2/mL^2$ have $n_x^2 + n_y^2 + n_z^2 = 6$. The following combinations of quantum numbers achieve this:

$$n_x = 2, \quad n_y = 1, \quad n_z = 1$$

$$n_x = 1, \quad n_y = 2, \quad n_z = 1$$

$$n_x = 1, \quad n_y = 1, \quad n_z = 2,$$

so the energy level is three-fold degenerate or its *degree of degeneracy* is 3.

Comment Note that, in specifying a quantum state, it matters *which* quantum number has *which* value.

Topic 8 — Continuity boundary conditions

Solution 8.1 $\psi(x)$ and $\mathrm{d}\psi/\mathrm{d}x$ are continuous functions at any point where the potential energy function $V(x)$ is finite, including the walls of a one-dimensional finite square well.

At the walls of a finite square well, $\psi(x)$ and $\mathrm{d}\psi/\mathrm{d}x$ are both continuous; at the walls of an infinite square well, $\psi(x)$ is continuous but $\mathrm{d}\psi/\mathrm{d}x$ is not.

Comments (1) As a finite square well becomes deeper and deeper, $\mathrm{d}\psi/\mathrm{d}x$ changes more and more rapidly in the vicinity of the walls of the well. In the limiting case of an infinite well, $\mathrm{d}\psi/\mathrm{d}x$ changes abruptly at the walls, corresponding to a discontinuity in the slope of the eigenfunction.

(2) These boundary conditions apply to energy eigenfunctions; they do not apply to all wave functions (see p. 69 of Book 1). For example, a wave function could have a discontinuous top-hat shape, as in Exercise 9.3 below.

Solution 8.2 We are told that $\psi_{\text{in}} = A\cos(kx)$ and $\psi_{\text{out}} = C\mathrm{e}^{-\alpha x}$ are the forms of the eigenfunction inside and outside the well respectively. Then continuity boundary conditions require that

$$\psi_{\text{in}}(L/2) = \psi_{\text{out}}(L/2) \quad \text{and} \quad \left.\frac{\mathrm{d}\psi_{\text{in}}}{\mathrm{d}x}\right|_{L/2} = \left.\frac{\mathrm{d}\psi_{\text{out}}}{\mathrm{d}x}\right|_{L/2}.$$

The first condition gives

$$A\cos\left(\frac{kL}{2}\right) = C\mathrm{e}^{-\alpha L/2}.$$

Differentiating the eigenfunction,

$$\frac{\mathrm{d}\psi_{\text{in}}}{\mathrm{d}x} = -kA\sin(kx) \quad \text{and} \quad \frac{\mathrm{d}\psi_{\text{out}}}{\mathrm{d}x} = -\alpha C\mathrm{e}^{-\alpha x},$$

so the second condition gives

$$-kA\sin\left(\frac{kL}{2}\right) = -\alpha C\mathrm{e}^{-\alpha L/2}.$$

Dividing the equation expressing the second boundary condition by that expressing the first, and cancelling a factor of -1, we conclude that

$$k \tan\left(\frac{kL}{2}\right) = \alpha.$$

Comment As the square well becomes very deep, α becomes very large, and the eigenfunction decays very rapidly outside the well. In the limiting case of an infinitely deep well, α tends to infinity and the above equation is satisfied by $kL/2 = \pi/2$, that is by $kL = \pi$, as expected.

Solution 8.3 Denote the interval $-L/2 < x < 0$ by Region 1, the interval $0 < x < L/2$ by Region 2 and elsewhere by Region 3. Then the time-independent Schrödinger equation in Region 1 is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x).$$

Using the form of the given eigenfunction appropriate for Region 1, this gives

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\big(A\cos(k_1x) + B\sin(k_1x)\big) = E\big(A\cos(k_1x) + B\sin(k_1x)\big).$$

Carrying out the differentiations, we obtain

$$\frac{\hbar^2k_1^2}{2m}\big(A\cos(k_1x) + B\sin(k_1x)\big) = E\big(A\cos(k_1x) + B\sin(k_1x)\big),$$

so

$$E = \frac{\hbar^2k_1^2}{2m}.$$

In Region 2, the time-independent Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V_0\psi(x) = E\psi(x),$$

and a similar argument gives

$$E = \frac{\hbar^2k_2^2}{2m} + V_0.$$

Equating these two expressions for the energy eigenvalue then gives

$$\frac{\hbar^2k_1^2}{2m} = \frac{\hbar^2k_2^2}{2m} + V_0,$$

which is the required relationship between k_1, k_2, V_0 and the mass m of the particle.

Comments (1) Note that we can apply the time-independent Schrödinger equation separately in Region 1 and Region 2, and our two expressions for the energy E can be equated because they refer to the same energy eigenvalue, E.

(2) In a sense, our final equation expresses basic energy accountancy: there is no potential energy in Region 1, so the kinetic energy in Region 1 ($\hbar^2k_1^2/2m$) is equal to the sum of the kinetic and potential energies in Region 2 ($\hbar^2k_2^2/2m + V_0$). However, this is talking rather loosely. The energy eigenvalue E refers to an energy eigenfunction which spreads throughout both Region 1 and Region 2. The particle is *not* confined to either Region 1 or Region 2; if it were, it would effectively be in a smaller well and its energy would be different!

Solution 8.4 The eigenfunction must be continuous at $x = -L/2$ (the boundary between Regions 1 and 3 as defined in the preceding solution) so

$$A\cos\left(\frac{-k_1L}{2}\right) + B\sin\left(\frac{-k_1L}{2}\right) = 0,$$

which simplifies to

$$\tan\left(\frac{k_1L}{2}\right) = \frac{A}{B}.$$

The eigenfunction must also be continuous at $x = L/2$ (the boundary between Regions 2 and 3) so

$$C\cos\left(\frac{k_2L}{2}\right) + D\sin\left(\frac{k_2L}{2}\right) = 0,$$

which simplifies to

$$\tan\left(\frac{k_2L}{2}\right) = -\frac{C}{D}.$$

At $x = 0$ (the boundary between Regions 1 and 2) both the eigenfunction and its derivative must be continuous, so

$$A\cos(0) + B\sin(0) = C\cos(0) + D\sin(0)$$

and

$$-k_1A\sin(0) + k_1B\cos(0) = -k_2C\sin(0) + k_2D\cos(0)$$

giving

$$A = C \quad \text{and} \quad k_1B = k_2D.$$

Combining the results obtained from all four continuity boundary conditions we conclude that

$$\tan\left(\frac{k_2L}{2}\right) = -\frac{C}{D} = -\frac{k_2}{k_1}\frac{A}{B} = -\frac{k_2}{k_1}\tan\left(\frac{k_1L}{2}\right),$$

which is the required relationship between k_1, k_2 and L.

Alternatively, we could write this as

$$\cot\left(\frac{k_2L}{2}\right) = -\frac{k_1}{k_2}\cot\left(\frac{k_1L}{2}\right),$$

Comment In the limiting case of an infinite square well with no step in it, we have $k_1 = k_2 = k$. From the first form of our final answer, we then obtain $\tan(kL/2) = 0$, and from the second form we obtain $\cot(kL/2) = 0$. These are equivalent to $\sin(kL/2) = 0$ and $\cos(kL/2) = 0$, which are the appropriate conditions for the odd and even energy eigenfunctions (respectively) of a symmetrical infinite square well.

Topic 9 — The overlap rule

Solution 9.1 (a) The probability p_i of measuring the energy eigenvalue E_i in a state described by the wave function $\Psi(x,t)$ is

$$p_i = \left|\int_{-\infty}^{\infty} \psi_i^*(x)\Psi(x,t)\,\mathrm{d}x\right|^2,$$

where $\psi_i(x)$ is the energy eigenfunction of the system corresponding to the eigenvalue E_i. Both $\psi_i(x)$ and $\Psi(x,t)$ are assumed to be normalized.

(b) If $\psi_i(x)$ is odd and $\Psi(x,t)$ is even, the integrand in the above integral is odd. This is integrated over a symmetric range, centred on the origin, so the integral is equal to zero. The probability of getting the corresponding eigenvalue E_i is then equal to zero.

Comment Note how the overlap rule works for energy measurements. We are looking for the probability of getting a given energy eigenvalue E_i when the energy of a system is measured. We need to know: (i) the wave function $\Psi(x,t)$ that describes the state of the system at the time of measurement and (ii) the energy eigenfunction $\psi_i(x)$ that corresponds to the energy eigenvalue E_i. This allows us to construct the overlap integral representing the probability amplitude for this measurement result. Don't forget to take the square of the modulus of the probability amplitude to find the corresponding probability.

Solution 9.2 If the system is in a state described by the energy eigenfunction $\psi_1(x)$, an energy measurement is certain to yield the corresponding eigenvalue, E_1. Consequently, the probability of obtaining any other eigenvalue, such as E_2, is equal to zero.

According to the overlap rule, the probability of obtaining the eigenvalue E_2 in the state $\psi_1(x)$ is

$$\text{probability} = \left| \int_{-\infty}^{\infty} \psi_2^*(x)\, \psi_1(x)\, \mathrm{d}x \right|^2,$$

which we know is equal to zero. Since the equation $|z|^2 = 0$ implies that $z = 0$, we conclude that

$$\int_{-\infty}^{\infty} \psi_2^*(x)\, \psi_1(x)\, \mathrm{d}x = 0,$$

confirming that $\psi_1(x)$ and $\psi_2(x)$ are orthogonal functions.

Comment Self-consistency of the overlap rule requires energy eigenfunctions with different eigenvalues to be orthogonal. However, the energy eigenfunctions are solutions of the time-independent Schrödinger equation, $\widehat{\mathrm{H}}\psi = E\psi$, which is the eigenvalue equation for the Hamiltonian operator, $\widehat{\mathrm{H}}$. This implies that there must be something special about the Hamiltonian operator in order for it to deliver eigenfunctions with the required orthogonal property. In Book 2, you will see that this special something is called the *Hermitian property* of the Hamiltonian operator, named after the French mathematician Charles Hermite.

Solution 9.3 The energy eigenfunction corresponding to the ground-state eigenvalue $E_1 = \pi^2\hbar^2/2mL^2$ is

$$\psi_1(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right),$$

so the probability of getting the value E_1 is

$$\begin{aligned} p_1 &= \left| \int_{-\infty}^{\infty} \psi_1^*(x) \Psi(x,0)\, \mathrm{d}x \right|^2 \\ &= \left| \int_{-w/2}^{w/2} \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right) \sqrt{\frac{1}{w}}\, \mathrm{d}x \right|^2 \\ &= \left| \sqrt{\frac{2}{wL}} \int_{-w/2}^{w/2} \cos\left(\frac{\pi x}{L}\right)\, \mathrm{d}x \right|^2. \end{aligned}$$

Rather than change variables in the integral, we can directly use the fact that

$$\int \cos(kx)\, \mathrm{d}x = \frac{1}{k} \sin(kx) + \text{arbitrary constant}$$

to obtain

$$\begin{aligned} p_1 &= \left| \sqrt{\frac{2}{wL}}\, \frac{L}{\pi} \left[\sin\left(\frac{\pi x}{L}\right)\right]_{-w/2}^{w/2} \right|^2 \\ &= \left| 2\sqrt{\frac{2L}{\pi^2 w}} \sin\left(\frac{\pi w}{2L}\right) \right|^2 \\ &= \frac{8L}{\pi^2 w} \sin^2\left(\frac{\pi w}{2L}\right). \end{aligned}$$

Comments (1) When substituting in the limits of integration, we have used the fact that, if $f(x) = -f(-x)$ is an odd function, then

$$\Big[f(x)\Big]_{-a}^{a} = 2f(a).$$

(2) The ratio w/L is dimensionless, so the final answer is dimensionless, as required for a probability.

(3) We can also check some values: at $w = L$, $p_1 = 8/\pi^2$, and as $w \to 0$, $\sin^2(\pi\omega/2L) \to (\pi\omega/2L)^2$ so $p_1 \to 0$. These values are reasonable because they both lie in the range between 0 and 1.

Topic 10 — The coefficient rule

Solution 10.1 In order for the wave function to be normalized, we must have

$$1 = \left|\frac{1}{2}\right|^2 + |\alpha|^2$$

so

$$|\alpha|^2 = \frac{3}{4},$$

and a possible value of α is $\sqrt{3}/2$.

This value is not unique and any choice of the form $\sqrt{3}e^{i\alpha}/2$, where α is real, would also produce a normalized wave function. In this case, however, different phases of α lead to different wave functions, representing different states. For example,

$$\frac{1}{2}\psi_1(x) + \frac{\sqrt{3}}{2}\psi_2(x) \quad \text{represents a different state from} \quad \frac{1}{2}\psi_1(x) - \frac{\sqrt{3}}{2}\psi_2(x),$$

with a different probability distribution for position measurements.

Comments (1) In a situation like this, normalization can be achieved using the coefficient rule directly; there is no need to write down or evaluate explicit normalization integrals.

(2) Distinguish this case (where the relative phase of two terms in a wave function matters) from the fact that an overall phase factor, multiplying the whole wave function, has no physical significance.

Solution 10.2 Normalization requires that

$$1 = |2N|^2 + |-\sqrt{5}N|^2 = 9|N|^2,$$

so we can choose $N = 1/3$.

The probability of getting energy E_1 is

$$p_1 = \left|\frac{2}{3}\right|^2 = \frac{4}{9},$$

and the probability of getting energy E_2 is

$$p_2 = \left|\frac{-\sqrt{5}}{3}\right|^2 = \frac{5}{9}.$$

The expectation value of the energy is

$$\langle E \rangle = p_1E_1 + p_2E_2 = \frac{4}{9}\varepsilon + \frac{5}{9}2\varepsilon = \frac{14}{9}\varepsilon.$$

Comments (1) We can check that $p_1 + p_2 = 5/9 + 4/9 = 1$, in agreement with the normalization rule for probability.

(2) In this case, the expectation value is not equal to either of the energy eigenvalues, but lies somewhere between them.

Solution 10.3 The normalization condition is

$$1 = \left|Ae^{-iE_1t/\hbar}\right|^2 + \left|-iAe^{-iE_2t/\hbar}\right|^2 = 2|A|^2$$

so a suitable value of A is $1/\sqrt{2}$.

The probability of measuring energy E_1 is

$$p_1 = \left|\frac{1}{\sqrt{2}}\,e^{-iE_1t/\hbar}\right|^2 = \frac{1}{2},$$

and the probability of measuring energy E_2 is

$$p_2 = \left|\frac{-i}{\sqrt{2}}\,e^{-iE_2t/\hbar}\right|^2 = \frac{1}{2},$$

so the expectation value of the energy is $\langle E\rangle = (E_1 + E_2)/2$.

Comment The fact that this expectation value is independent of time, even though the wave function and other expectation values depend on time, is related to the principle of conservation of energy.

Solution 10.4 (a) The normalization condition is

$$\left|a_1 \mathrm{e}^{-\mathrm{i}E_1 t/\hbar}\right|^2 + \left|a_2 \mathrm{e}^{-\mathrm{i}E_2 t/\hbar}\right|^2 + \left|a_3 \mathrm{e}^{-\mathrm{i}E_3 t/\hbar}\right|^2 = |a_1|^2 + |a_2|^2 + |a_3|^2 = 1.$$

(b) No. It never makes a difference to multiply a whole wave function by a phase factor (a complex number of unit modulus).

(c) Yes. This will affect the interference between different terms in $\Psi(x,t)$.

(d) No. The expectation value of the energy is

$$\langle E\rangle = |a_1|^2 E_1 + |a_2|^2 E_2 + |a_3|^2 E_3,$$

which is unchanged by reversing the sign of a_1.

Comment Reversing the sign of a_1 alone changes the state of the system (witnessed, for example, by the change in the expectation value of x) but the original state and the new state share the probability distribution for energy. So, in general, the probability distribution for energy is insufficient to specify a quantum state.

Topic 11 — The sandwich integral rule

Solution 11.1 (a) The sandwich integral rule states that, for a one-dimensional system described by the normalized wave function $\Psi(x,t)$, the expectation value at time t of an observable A is

$$\langle A\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, \widehat{\mathrm{A}}\Psi(x,t)\,\mathrm{d}x,$$

where $\widehat{\mathrm{A}}$ is the quantum-mechanical operator corresponding to the observable A.

(b) The expectation value of position is

$$\begin{aligned}\langle x\rangle &= \int_{-\infty}^{\infty} A^*\mathrm{e}^{-\alpha x^2} x A\mathrm{e}^{-\alpha x^2}\,\mathrm{d}x \\ &= |A|^2 \int_{-\infty}^{\infty} x\,\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x \\ &= 0,\end{aligned}$$

because the integrand is an odd function and the range of integration is symmetrical about $x = 0$.

The expectation value of momentum is

$$\begin{aligned}\langle p_x\rangle &= \int_{-\infty}^{\infty} A^*\mathrm{e}^{-\alpha x^2}\left(-\mathrm{i}\hbar\frac{\partial}{\partial x}A\mathrm{e}^{-\alpha x^2}\right)\mathrm{d}x \\ &= -\mathrm{i}\hbar|A|^2 \int_{-\infty}^{\infty} \mathrm{e}^{-\alpha x^2}\left(-2\alpha x\mathrm{e}^{-\alpha x^2}\right)\mathrm{d}x \\ &= 2\mathrm{i}\hbar\alpha|A|^2 \int_{-\infty}^{\infty} x\,\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x \\ &= 0,\end{aligned}$$

because the integrand is odd and the integral is over a range centred on $x = 0$.

Comments (1) When using the sandwich integral rule, allow the relevant operator to act on the wave function $\Psi(x,t)$ before multiplying by the complex conjugate $\Psi^*(x,t)$, collecting terms and integrating. This does not matter much in part (a) but is more important in part (b).

(2) The integral in part (b) can be evaluated more simply by noting that $-\mathrm{i}\hbar\partial/\partial x$ is an odd operator (changing sign when $x \to -x$) while $\mathrm{e}^{-\alpha x^2}$ is an even function. This shows that the integrand is an odd function (without the need to carry out any differentiation).

Solution 11.2 We have

$$\begin{aligned}\langle x^2\rangle &= \int_{-\infty}^{\infty} \psi_n^*(x)\, x^2 \psi_n(x)\,\mathrm{d}x \\ &= \frac{2}{L}\int_0^L x^2\, \sin^2\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x.\end{aligned}$$

Change variables to $u = n\pi x/L$. Then $x = 0$ corresponds to $u = 0$ and $x = L$ corresponds to $u = n\pi$. Also, $x = (L/n\pi)\,u$ and $\mathrm{d}x = (L/n\pi)\,\mathrm{d}u$, so

$$\langle x^2\rangle = \frac{2}{L}\left(\frac{L}{n\pi}\right)^3 \int_0^{n\pi} u^2 \sin^2 u\,\mathrm{d}u.$$

Using the standard integral given in the question, we conclude that

$$\begin{aligned}\langle x^2\rangle &= \frac{2}{L}\left(\frac{L}{n\pi}\right)^3 \frac{n\pi}{12}(2n^2\pi^2 - 3) \\ &= \frac{L^2}{6}\left(2 - \frac{3}{n^2\pi^2}\right).\end{aligned}$$

Comments (1) The answer is dimensionally correct because the expectation value of x^2 must have the units of length^2.

(2) In the limit of very high quantum numbers ($n \to \infty$) we get $\langle x^2\rangle \to L^2/3$. Compare this with the corresponding classical result. In classical physics, the particle is equally likely to be found anywhere inside the box, so the probability density has the constant value $1/L$ for $0 < x < L$, giving a classical expectation value for x^2 of $\int_0^L x^2(1/L)\,\mathrm{d}x = L^2/3$. In the limit of very high quantum numbers, the quantum result approaches the classical result; this agrees with the correspondence principle (Book 1 p. 135).

Solution 11.3 In the given state, the expectation value of p_x^2 is

$$\begin{aligned}\langle p_x^2\rangle &= \frac{1}{\sqrt{\pi}a}\int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2a^2}\, \widehat{\mathrm{p}}_x^2\, \mathrm{e}^{-x^2/2a^2}\,\mathrm{d}x \\ &= -\frac{\hbar^2}{\sqrt{\pi}a}\int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2a^2}\, \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\mathrm{e}^{-x^2/2a^2}\right)\,\mathrm{d}x.\end{aligned}$$

Using the derivative given in the question, we obtain

$$\begin{aligned}\langle p_x^2\rangle &= -\frac{\hbar^2}{\sqrt{\pi}a}\int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2a^2}\, \frac{1}{a^2}\left(\frac{x^2}{a^2} - 1\right)\mathrm{e}^{-x^2/2a^2}\,\mathrm{d}x \\ &= -\frac{\hbar^2}{\sqrt{\pi}a^3}\int_{-\infty}^{\infty}\left(\frac{x^2}{a^2} - 1\right)\mathrm{e}^{-x^2/a^2}\,\mathrm{d}x.\end{aligned}$$

We change variables to $u = x/a$ and use the standard integrals given in the question. Then $x = au$ and $\mathrm{d}x = a\,\mathrm{d}u$. The limits of integration remain $\pm\infty$, so

$$\begin{aligned}\langle p_x^2\rangle &= -\frac{\hbar^2}{\sqrt{\pi}a^3}\left[a\int_{-\infty}^{\infty} u^2\mathrm{e}^{-u^2}\,\mathrm{d}u - a\int_{-\infty}^{\infty}\mathrm{e}^{-u^2}\,\mathrm{d}u\right] \\ &= -\frac{\hbar^2}{\sqrt{\pi}a^2}\left[\frac{\sqrt{\pi}}{2} - \sqrt{\pi}\right] \\ &= \frac{\hbar^2}{2a^2}.\end{aligned}$$

Comment As the constant a becomes smaller, the wave function becomes more narrowly peaked around $x = 0$, and our answer shows that $\langle p_x^2\rangle$ increases. This can be understood as follows. When the wave function is represented as a linear combination of plane waves, a greater spread of k values is needed to produce a narrow peak rather than a broad peak. This corresponds to a greater spread in momentum values $p_x = \hbar k$, and so to a greater expectation value of p_x^2. The greater spread of momentum values is also consistent with the Heisenberg uncertainty principle.

Solution 11.4 The expectation value is given by

$$\left\langle e^{-\lambda^2 x^2} \right\rangle = \frac{1}{\sqrt{\pi} a} \int_{-\infty}^{\infty} e^{-x^2/2a^2}\, e^{-\lambda^2 x^2}\, e^{-x^2/2a^2}\, dx.$$

We can collect together all the exponential factors to obtain

$$\left\langle e^{-\lambda^2 x^2} \right\rangle = \frac{1}{\sqrt{\pi} a} \int_{-\infty}^{\infty} e^{-(\lambda^2 + 1/a^2)x^2}\, dx.$$

Using the standard integral given in the question, with

$$\alpha = \lambda^2 + 1/a^2 = \frac{(1 + \lambda^2 a^2)}{a^2}$$

we get

$$\left\langle e^{-\lambda^2 x^2} \right\rangle = \frac{1}{\sqrt{\pi} a} \times \frac{\sqrt{\pi} a}{(1 + \lambda^2 a^2)^{1/2}} = (1 + \lambda^2 a^2)^{-1/2}.$$

Comments (1) The expectation value of any function of x could be calculated in a similar way.

(2) One way of checking this answer is to consider the limiting case $\lambda = 0$. In this case, $e^{-\lambda^2 x^2} = 1$, so the sandwich integral becomes equal to the normalization integral, which is equal to 1. Our final answer gives this value for $\lambda = 0$.

Topic 12 — Uncertainties and the uncertainty principle

Solution 12.1 Energy $E_1 = \varepsilon$ occurs with probability

$$p_1 = \left| \frac{\sqrt{3}}{2} \right|^2 = \frac{3}{4}.$$

Energy $E_2 = 2\varepsilon$ occurs with probability

$$p_2 = \left| \frac{i}{2} \right|^2 = \frac{1}{4}.$$

The expectation value of the energy is therefore

$$\langle E \rangle = \frac{3}{4}\varepsilon + \frac{1}{4} 2\varepsilon = \frac{5}{4}\varepsilon.$$

The expectation value of the square of the energy is

$$\langle E^2 \rangle = \frac{3}{4}\varepsilon^2 + \frac{1}{4}(2\varepsilon)^2 = \frac{7}{4}\varepsilon^2.$$

So

$$\begin{aligned}(\Delta E)^2 &= \langle E^2 \rangle - \langle E \rangle^2 \\ &= \frac{7}{4}\varepsilon^2 - \frac{25}{16}\varepsilon^2 = \frac{3}{16}\varepsilon^2\end{aligned}$$

and the uncertainty of the energy is

$$\Delta E = \frac{\sqrt{3}}{4}\varepsilon.$$

Comments (1) The probabilities are found by taking the square of the modulus of the coefficients in the wave function. These probabilities turn out to lie in the range from 0 to 1, as required.

(2) The expectation value of E is a weighted sum of the possible values of E, with each allowed energy value multiplied by its corresponding probability. The expectation value of E^2 can be written as a similar sum with the *same* probabilities, which now multiply the *squares* of the values of E. This works because, to find the square of the energy in any particular measurement, we can measure the energy value E and then take its square.

(3) It is convenient to calculate the square of the uncertainty first, and then take the square root.

Solution 12.2 (a) The square of the uncertainty in x is

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = 2.0\,\text{nm}^2 - (1.0\,\text{nm})^2 = 1.0\,\text{nm}^2,$$

so

$$\Delta x = 1.0\,\text{nm}.$$

(b) The minimum value of Δp_x, consistent with the above value of Δx is

$$(\Delta p_x)_{\text{min}} = \frac{\hbar}{2\,\Delta x} = \frac{1.06 \times 10^{-34}\,\text{J s}}{2 \times 10^{-9}\,\text{m}} = 5.3 \times 10^{-26}\,\text{kg m s}^{-1}.$$

The minimum Δp_y consistent with the given value of Δx is zero.

Comment The Heisenberg uncertainty principle applies to position and momentum components along the same axis. There is no uncertainty principle for a position component along one axis and a momentum component along a perpendicular axis.

Topic 13 — Harmonic oscillators

Solution 13.1 We have

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\mathrm{e}^{-\alpha x^2}\right) &= \frac{\mathrm{d}}{\mathrm{d}x}\left(-2\alpha x\mathrm{e}^{-\alpha x^2}\right)\\ &= (-2\alpha + 4\alpha^2 x^2)\mathrm{e}^{-\alpha x^2}.\end{aligned}$$

Substituting into the time-independent Schrödinger equation, we obtain

$$-\frac{\hbar^2}{2m}(-2\alpha + 4\alpha^2 x^2)\mathrm{e}^{-\alpha x^2} + \tfrac{1}{2}Cx^2\mathrm{e}^{-\alpha x^2} = E\mathrm{e}^{-\alpha x^2}.$$

Dividing through by $\mathrm{e}^{-\alpha x^2}$ and rearranging, we conclude that

$$\left(-\frac{4\hbar^2\alpha^2}{2m} + \frac{1}{2}C\right)x^2 + \left(\frac{\hbar^2\alpha}{m} - E\right) = 0.$$

For this equation to be true for all x, each of the terms in round brackets must vanish separately, so we have

$$\frac{4\hbar^2\alpha^2}{2m} = \frac{1}{2}C \quad \text{and} \quad \frac{\hbar^2\alpha}{m} = E.$$

Hence

$$\alpha = \frac{\sqrt{mC}}{2\hbar} \quad \text{and} \quad E = \frac{\hbar^2}{m}\frac{\sqrt{mC}}{2\hbar} = \frac{\hbar}{2}\sqrt{\frac{C}{m}}.$$

Comment Notice that two pieces of information can be extracted from a single equation. This is because the time-independent Schrödinger equation is valid for all values of x. Putting $x = 0$ gives a relationship between E and α. Using this relationship and considering the time-independent Schrödinger equation for $x \neq 0$ then gives a relationship between α and C.

Solution 13.2 The energy levels of a simple harmonic oscillator are given by

$$E = (n + \tfrac{1}{2})\hbar\omega_0 \quad \text{for } n = 0, 1, 2, \ldots,$$

where ω_0 is the classical angular frequency. The zero-point energy is the lowest possible energy above the bottom of the potential well:

$$E_{\text{zero-point}} = E_0 = \tfrac{1}{2}\hbar\omega_0.$$

The radiative transitions in a harmonic oscillator are subject to a selection rule that restricts Δn to ± 1. So a radiative transition from a state with $n = 5$ to a state of lower energy can only be to the state $n = 4$, and the energy

of the photon emitted is

$$\begin{aligned}E_{\text{photon}} &= (5+\tfrac{1}{2})\hbar\omega_0 - (4+\tfrac{1}{2})\hbar\omega_0\\ &= \hbar\omega_0\\ &= 2E_{\text{zero-point}}\\ &= 3.0\,\text{eV}.\end{aligned}$$

For electromagnetic radiation, $E = hf$ and $c = f\lambda$, so the wavelength of the emitted light is

$$\lambda = \frac{c}{f} = \frac{hc}{E} = \frac{6.63\times10^{-34}\,\text{J s}\times 3.00\times10^{8}\,\text{m s}^{-1}}{3.0\times1.60\times10^{-19}\,\text{J}} = 4.1\times10^{-7}\,\text{m}.$$

Comment Because of the selection rule, and the fact that the energy levels of a harmonic oscillator are equally spaced, a harmonic oscillator produces only one spectral line no matter how much it is excited. Harmonic oscillators are unique in this respect; atoms have much more complicated spectra.

Solution 13.3 In terms of raising and lowering operators

$$\widehat{\mathrm{x}} = \frac{a}{\sqrt{2}}\left(\widehat{\mathrm{A}} + \widehat{\mathrm{A}}^\dagger\right) \quad \text{and} \quad \widehat{\mathrm{p}}_x = \frac{-\mathrm{i}\hbar}{\sqrt{2}a}\left(\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger\right).$$

Combining these results and multiplying out the brackets (whilst preserving the order of operators) gives

$$\begin{aligned}\widehat{\mathrm{x}}\,\widehat{\mathrm{p}}_x &= \frac{-\mathrm{i}\hbar}{2}\left(\widehat{\mathrm{A}} + \widehat{\mathrm{A}}^\dagger\right)\left(\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger\right)\\ &= \frac{-\mathrm{i}\hbar}{2}\left(\widehat{\mathrm{A}}\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger + \widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}} - \widehat{\mathrm{A}}\widehat{\mathrm{A}}^\dagger\right)\\ &= \frac{-\mathrm{i}\hbar}{2}\left(\widehat{\mathrm{A}}\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger - 1\right),\end{aligned}$$

where we have used the commutation relation $\widehat{\mathrm{A}}\widehat{\mathrm{A}}^\dagger - \widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}} = 1$.

So, in a harmonic oscillator energy eigenstate with quantum number n,

$$\langle\widehat{\mathrm{x}}\,\widehat{\mathrm{p}}_x\rangle = -\frac{\mathrm{i}\hbar}{2}\int_{-\infty}^{\infty}\psi_n^*(x)\left(\widehat{\mathrm{A}}\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger - 1\right)\psi_n(x)\,\mathrm{d}x.$$

This splits into three integrals. We have

$$\int_{-\infty}^{\infty}\psi_n^*(x)\,\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger\psi_n(x)\,\mathrm{d}x = \alpha\int_{-\infty}^{\infty}\psi_n^*(x)\,\psi_{n+2}(x)\,\mathrm{d}x = 0,$$

where α is a proportionality constant. The integral is equal to 0 because $\psi_n(x)$ and $\psi_{n+2}(x)$ are orthogonal.

For $n = 0$ or $n = 1$, we have $\widehat{\mathrm{A}}\widehat{\mathrm{A}}\psi_n(x) = 0$, while for $n \geq 2$,

$$\int_{-\infty}^{\infty}\psi_n^*(x)\,\widehat{\mathrm{A}}\widehat{\mathrm{A}}\psi_n(x)\,\mathrm{d}x = \beta\int_{-\infty}^{\infty}\psi_n^*(x)\,\psi_{n-2}(x)\,\mathrm{d}x = 0,$$

where β is another proportionality constant. Again, the integral is equal to zero because $\psi_n(x)$ and $\psi_{n-2}(x)$ are orthogonal.

We therefore conclude that

$$\begin{aligned}\langle\widehat{\mathrm{x}}\,\widehat{\mathrm{p}}_x\rangle &= +\frac{\mathrm{i}\hbar}{2}\int_{-\infty}^{\infty}\psi_n^*(x)\,\psi_n(x)\,\mathrm{d}x\\ &= \frac{\mathrm{i}\hbar}{2}\end{aligned}$$

because $\psi_n(x)$ is normalized.

Comments (1) When multiplying out brackets involving raising and lowering operators it is essential to preserve the order of the operators because they do not commute.

(2) When arguing that a given integral involving raising and lowering operators is equal to zero, you need not give explicit values for proportionality factors such as α and β above.

Solution 13.4 (a) Multiplying out the brackets (whilst preserving operator order in products) we obtain

$$\begin{aligned}\big(\widehat{\mathrm{A}}+\widehat{\mathrm{A}}^\dagger\big)^2+\big(\widehat{\mathrm{A}}-\widehat{\mathrm{A}}^\dagger\big)^2 &= \big(\widehat{\mathrm{A}}\widehat{\mathrm{A}}+\widehat{\mathrm{A}}\widehat{\mathrm{A}}^\dagger+\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}+\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger\big)\\ &\quad+\big(\widehat{\mathrm{A}}\widehat{\mathrm{A}}-\widehat{\mathrm{A}}\widehat{\mathrm{A}}^\dagger-\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}+\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger\big)\\ &= 2\big(\widehat{\mathrm{A}}\widehat{\mathrm{A}}+\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger\big).\end{aligned}$$

So the integral given in the question becomes

$$I=2\int_{-\infty}^{\infty}\psi_n^*(x)\,\widehat{\mathrm{A}}\widehat{\mathrm{A}}\psi_n(x)\,\mathrm{d}x+2\int_{-\infty}^{\infty}\psi_n^*(x)\,\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}^\dagger\psi_n(x)\,\mathrm{d}x.$$

Both terms on the right-hand side are equal to zero (by the argument given in the answer to the previous question).

(b) Using the formulae given in the question, we find that, in the state ψ_n,

$$\frac{1}{a^2}\langle x^2\rangle=\frac{1}{2}\int_{-\infty}^{\infty}\psi_n^*(x)\big(\widehat{\mathrm{A}}+\widehat{\mathrm{A}}^\dagger\big)^2\psi_n(x)\,\mathrm{d}x$$

$$\frac{a^2}{\hbar^2}\langle p_x^2\rangle=-\frac{1}{2}\int_{-\infty}^{\infty}\psi_n^*(x)\big(\widehat{\mathrm{A}}-\widehat{\mathrm{A}}^\dagger\big)^2\psi_n(x)\,\mathrm{d}x.$$

Subtracting these two equations then gives

$$\frac{1}{a^2}\langle x^2\rangle-\frac{a^2}{\hbar^2}\langle p_x^2\rangle=\frac{1}{2}\int_{-\infty}^{\infty}\psi_n^*(x)\Big[\big(\widehat{\mathrm{A}}+\widehat{\mathrm{A}}^\dagger\big)^2+\big(\widehat{\mathrm{A}}-\widehat{\mathrm{A}}^\dagger\big)^2\Big]\psi_n(x)\,\mathrm{d}x=0,$$

by the result derived in part (a). Hence $\langle x^2\rangle/a^2=(a^2/\hbar^2)\langle p_x^2\rangle$, as required.

Using $a^4=\hbar^2/mC$, we can rewrite this result as

$$\frac{1}{2}C\langle x^2\rangle=\frac{1}{2m}\langle p_x^2\rangle,$$

which shows that the expectation values of the potential and kinetic energies are equal in any energy eigenstate of a harmonic oscillator (i.e any stationary state of the oscillator, represented by an energy eigenfunction).

Comment This quantum-mechanical result is closely related to a similar result in classical physics. For a classical harmonic oscillator, the time-average of the kinetic energy is equal to the time-average of the potential energy when both are averaged over a whole number of cycles.

Topic 14 — Bound-state wave packets

Solution 14.1 (a) At time t, the wave packet is

$$\begin{aligned}\Psi(x,t)&=\frac{1}{\sqrt{2}}\left(\psi_1(x)\,\mathrm{e}^{-\mathrm{i}E_1t/\hbar}+\mathrm{i}\,\psi_2(x)\,\mathrm{e}^{-\mathrm{i}E_2t/\hbar}\right)\\ &=\frac{1}{\sqrt{2}}\left(\psi_1(x)\,\mathrm{e}^{-3\mathrm{i}\omega_0t/2}+\mathrm{i}\,\psi_2(x)\,\mathrm{e}^{-5\mathrm{i}\omega_0t/2}\right)\\ &=\frac{\mathrm{e}^{-3\mathrm{i}\omega_0t/2}}{\sqrt{2}}\left(\psi_1(x)+\mathrm{i}\,\psi_2(x)\,\mathrm{e}^{-\mathrm{i}\omega_0t}\right).\end{aligned}$$

(b) To see if there is a time when $\Psi(x,t)$ is orthogonal to the initial wave function, $\Psi(x,0)$, we consider

$$\begin{aligned}\int_{-\infty}^{\infty}\Psi^*(x,0)\,\Psi(x,t)\,\mathrm{d}x&=\frac{\mathrm{e}^{-3\mathrm{i}\omega_0t/2}}{2}\int_{-\infty}^{\infty}\big[\psi_1(x)+\mathrm{i}\,\psi_2(x)\big]^*\big[\psi_1(x)+\mathrm{i}\,\psi_2(x)\,\mathrm{e}^{-\mathrm{i}\omega_0t}\big]\,\mathrm{d}x\\ &=\frac{\mathrm{e}^{-3\mathrm{i}\omega_0t/2}}{2}\int_{-\infty}^{\infty}\big[\psi_1^*(x)-\mathrm{i}\,\psi_2^*(x)\big]\big[\psi_1(x)+\mathrm{i}\,\psi_2(x)\,\mathrm{e}^{-\mathrm{i}\omega_0t}\big]\,\mathrm{d}x.\end{aligned}$$

Multiplying out the brackets and remembering that energy eigenfunctions with different energy eigenvalues are orthogonal gives

$$\begin{aligned}\int_{-\infty}^{\infty} \Psi^*(x,0)\,\Psi(x,t)\,\mathrm{d}x &= \frac{\mathrm{e}^{-3\mathrm{i}\omega_0 t/2}}{2}\left[\int_{-\infty}^{\infty} \psi_1^*(x)\,\psi_1(x)\,\mathrm{d}x + \psi_2^*(x)\,\psi_2(x)\,\mathrm{e}^{-\mathrm{i}\omega_0 t}\right]\mathrm{d}x \\ &= \frac{\mathrm{e}^{-3\mathrm{i}\omega_0 t/2}}{2}\left[1+\mathrm{e}^{-\mathrm{i}\omega_0 t}\right],\end{aligned}$$

where we have used the fact that $\psi_1(x)$ and $\psi_2(x)$ are normalized.

The overlap integral between $\Psi(x,t)$ and $\Psi(x,0)$ is equal to zero when $\mathrm{e}^{-\mathrm{i}\omega_0 t} = -1$. Since $\mathrm{e}^{-in\pi} = -1$ for $n = 1, 3, 5, \ldots$, the positive values of t for which the overlap integral is vanishes are: $t = \pi/\omega_0, 3\pi/\omega_0, \ldots$.

Comments (1) When an initial wave function $\Psi(x,0)$ is given as a sum of energy eigenfunctions, the corresponding time-dependent wave function $\Psi(x,t)$ is constructed by inserting appropriate time-dependent phase factors. Each energy eigenfunction has a different phase factor. Because these vary at different rates, the shape of the wave function can vary in an interesting way.

(2) To establish orthogonality, we must evaluate an integral: the calculation in part (b) would not be valid without integral signs.

Solution 14.2 (a) The probability density is

$$\begin{aligned}\Psi^*(x,t)\,\Psi(x,t) &= \frac{1}{2}\left(\psi_0^*(x)\,\mathrm{e}^{\mathrm{i}E_0 t/\hbar} + \psi_2^*(x)\,\mathrm{e}^{\mathrm{i}E_2 t/\hbar}\right)\left(\psi_0(x)\,\mathrm{e}^{-\mathrm{i}E_0 t/\hbar} + \psi_2(x)\,\mathrm{e}^{-\mathrm{i}E_2 t/\hbar}\right) \\ &= \frac{1}{2}\Big(|\psi_0(x)|^2 + |\psi_2(x)|^2 + \psi_0^*(x)\,\psi_2(x)\,\mathrm{e}^{\mathrm{i}(E_0-E_2)t/\hbar} \\ &\qquad + \psi_2^*(x)\,\psi_0(x)\,\mathrm{e}^{\mathrm{i}(E_2-E_0)t/\hbar}\Big).\end{aligned}$$

This is periodic with period T where $(E_2 - E_0)T/\hbar = 2\pi$. So

$$T = \frac{2\pi\hbar}{E_2 - E_0} = \frac{2\pi\hbar}{2\hbar\omega_0} = \frac{\pi}{\omega_0}.$$

(b) $\psi_0(x)$ and $\psi_2(x)$ are harmonic oscillator energy eigenfunctions with $n = 0$ and $n = 2$; these are both even functions of x, so $\Psi(-x,t) = \Psi(x,t)$ at all times. Consequently, the probability density is an even function of x and the particle is always equally likely to be found in the regions $x < 0$ and $x > 0$. The motion of this wave packet does not correspond to a classical to-and-fro motion, but to a symmetric breathing in and out (in which the probability density undergoes one cycle of oscillation in half the classical period of oscillation).

Comments (1) By contrast with the previous exercise, calculations of the probability density involve no integration.

(2) The time-dependence of the probability density arises from the cross-product terms when we multiply out the brackets. For some wave packets, such as that considered here, the period of oscillation can be shorter than the classical period.

Topic 15 — Free-particle wave packets

Solution 15.1 At any later time, we have

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)\,\mathrm{e}^{\mathrm{i}(kx - E_k t/\hbar)}\,\mathrm{d}k,$$

where $E_k = \hbar^2 k^2/2m$.

$A(k)$ is the momentum amplitude function. The probability of finding the momentum to be in a small range of width $\hbar\,\delta k$, centred on $\hbar k$ is $|A(k)|^2\,\delta k$. More generally, the probability of finding the momentum to be in the range from $\hbar k_1$ to $\hbar k_2$ is

$$\text{probability} = \int_{k_1}^{k_2} |A(k)|^2\,\mathrm{d}k.$$

Comments (1) The method used to find the time-dependent wave function is similar to that described in Exercise 14.1 for a harmonic-oscillator wave packet. The only difference is that we now have an integral over k rather than a discrete sum (and, of course, we must use the energy eigenvalues for a free particle, $E_k = \hbar^2 k^2/2m$).

(2) The interpretation of $A(k)$ is based on Born's rule for momentum, which is closely analogous to Born's rule (for position). Note, however, that $A(k)$ is expressed as a function of the wave number k, while the momentum is $p_x = \hbar k$. This means you must remember to include various factors of $\hbar$ in the *descriptions* of momenta and momentum ranges, but *not* in the formulae $|A(k)|^2\,\delta k$ or $\int_{k_1}^{k_2} |A(k)|^2\,\mathrm{d}k$.

Solution 15.2 (a) The momentum amplitude function is

$$\begin{aligned}
A(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \int_{-L/2}^{L/2} \frac{1}{\sqrt{L}}\,\mathrm{e}^{\mathrm{i}\alpha x}\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi L}} \int_{-L/2}^{L/2} \mathrm{e}^{\mathrm{i}(\alpha-k)x}\,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi L}} \left[\frac{\mathrm{e}^{\mathrm{i}(\alpha-k)x}}{\mathrm{i}(\alpha-k)}\right]_{-L/2}^{L/2} \\
&= \frac{1}{\sqrt{2\pi L}}\, \frac{\mathrm{e}^{\mathrm{i}(\alpha-k)L/2} - \mathrm{e}^{-\mathrm{i}(\alpha-k)L/2}}{\mathrm{i}(\alpha-k)} \\
&= \sqrt{\frac{2}{\pi L}}\, \frac{\sin\left[(\alpha-k)L/2\right]}{\alpha-k},
\end{aligned}$$

where we have used the identity $\sin\theta = (\mathrm{e}^{\mathrm{i}\theta} - \mathrm{e}^{-\mathrm{i}\theta})/2\mathrm{i}$.

(b) The probability of measuring a momentum between $-\hbar\alpha$ and $+\hbar\alpha$ is

$$\begin{aligned}
\text{probability} &= \int_{-\alpha}^{+\alpha} |A(k)|^2\,\mathrm{d}k \\
&= \frac{2}{\pi L} \int_{-\alpha}^{+\alpha} \frac{\sin^2[(\alpha-k)L/2]}{(\alpha-k)^2}\,\mathrm{d}k.
\end{aligned}$$

We change the variable of integration from k to $u = (\alpha - k)L/2$. Then $(\alpha - k) = 2u/L$ and $\mathrm{d}k = -(2/L)\mathrm{d}u$. Also, $k = -\alpha$ corresponds to $u = \alpha L$ and $k = +\alpha$ corresponds to $u = 0$, so we have

$$\begin{aligned}
\text{probability} &= \frac{2}{\pi L} \int_{\alpha L}^{0} \frac{\sin^2 u}{(2u/L)^2} \times -\frac{2}{L}\mathrm{d}u \\
&= \frac{1}{\pi} \int_{0}^{\alpha L} \frac{\sin^2 u}{u^2}\,\mathrm{d}u.
\end{aligned}$$

For the special case $\alpha = 1/L$, the standard integral in the question gives

$$\text{probability} = \frac{1}{\pi} \int_0^1 \frac{\sin^2 u}{u^2}\,\mathrm{d}u = \frac{0.897}{\pi} = 0.286.$$

Comment The given wave function can be described as a *truncated plane wave* because it looks like a plane wave in the region between $-L/2$ and $L/2$ and vanishes outside this region. In spite of this fact, it corresponds to a spread of momenta $\hbar k$ with a probability distribution given by $|A(k)|^2$, which is nothing like the single momentum value associated with a plane wave that extends indefinitely. The reason for this is as follows. If the wave function is represented as a linear combination of $\mathrm{e}^{\mathrm{i}kx}$ terms, a broad range of different k values is needed to get the required complete cancellation in the region $|x| > L/2$. The different k values correspond to different momenta. In accordance with the Heisenberg uncertainty principle, the momentum uncertainty increases as L decreases.

Solution 15.3 (a) The function $\Psi_{\text{dB}}(x,t)$ cannot be normalized. It corresponds to a particle with a definite value of momentum and an infinite uncertainty in position. Such a particle could be found with any value of x between $-\infty$ and $+\infty$, which is not realistic.

(b) The probability that a momentum measurement will yield a value between $p_1 = \hbar k_1$ and $p_2 = \hbar k_2$ is

$$\int_{k_1}^{k_2} |A(k)|^2 \, \mathrm{d}k.$$

The condition for normalization is that

$$\int_{-\infty}^{\infty} |A(k)|^2 \, \mathrm{d}k = 1.$$

Comment In physical terms, the above normalization condition expresses the fact that a measurement of the momentum is bound to give some value between $-\infty$ and $+\infty$. A mathematical result known as Plancherel's theorem (or Parseval's theorem) guarantees that this condition also gives

$$\int_{-\infty}^{\infty} |\Psi_{\text{dB}}(x,t)|^2 \, \mathrm{d}x = 1,$$

so the wave function is normalized.

Topic 16 — Ehrenfest's theorem

Solution 16.1 Ehrenfest's theorem states that

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{\langle p_x\rangle}{m}$$

and

$$\frac{\mathrm{d}\langle p_x\rangle}{\mathrm{d}t} = -\left\langle \frac{\partial V}{\partial x} \right\rangle.$$

If $V(x) = mgx$, then $\partial V/\partial x = mg$ and

$$\frac{\mathrm{d}\langle p_x\rangle}{\mathrm{d}t} = -mg.$$

Hence,

$$\frac{\mathrm{d}^2\langle x\rangle}{\mathrm{d}t^2} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\langle p_x\rangle}{m}\right) = \frac{1}{m}\frac{\mathrm{d}\langle p_x\rangle}{\mathrm{d}t} = -\frac{mg}{m} = -g.$$

Comment This is the quantum-mechanical version of the familiar classical statement that close to the Earth, in the absence of air-resistance, particles move with a constant downward acceleration of magnitude g. The quantum result differs from the classical one because it involves an expectation value. For a particle dropped from rest, the time of fall would have a probability distribution associated with the spatial spread of the particle's wave packet.

Topic 17 — Scattering and tunnelling

Solution 17.1 Continuity of $\psi(x)$ at $x = 0$ gives

$$A + B = C.$$

Continuity of $\mathrm{d}\psi/\mathrm{d}x$ at $x = 0$ gives

$$\mathrm{i}k_1(A - B) = \mathrm{i}k_2 C.$$

So, eliminating C,

$$A + B = \frac{k_1}{k_2}(A - B).$$

Hence

$$B(k_1/k_2 + 1) = A(k_1/k_2 - 1)$$

and

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}.$$

Comment As a quick check, note that $B/A = 0$ when $k_1 = k_2$. Sensibly enough, this means there is no reflection when there is no step.

Solution 17.2 Continuity of $\psi(x)$ at $x = 0$ gives

$$A + B = C.$$

Continuity of $\mathrm{d}\psi/\mathrm{d}x$ at $x = 0$ gives

$$\mathrm{i}k_1(A - B) = -\alpha C.$$

So, eliminating C,

$$A + B = -\frac{\mathrm{i}k_1}{\alpha}(A - B).$$

Hence

$$B(\mathrm{i}k_1/\alpha - 1) = A(\mathrm{i}k_1/\alpha + 1)$$

and

$$\frac{B}{A} = \frac{\mathrm{i}k_1/\alpha + 1}{\mathrm{i}k_1/\alpha - 1} = \frac{\mathrm{i}k_1 + \alpha}{\mathrm{i}k_1 - \alpha}.$$

So

$$\left|\frac{B}{A}\right|^2 = \frac{(\mathrm{i}k_1 + \alpha)}{(\mathrm{i}k_1 - \alpha)} \times \frac{(-\mathrm{i}k_1 + \alpha)}{(-\mathrm{i}k_1 - \alpha)} = \frac{k_1^2 + \alpha^2}{k_1^2 + \alpha^2} = 1.$$

Comment $|B/A|^2$ is the reflection coefficient, so the physical interpretation of this result is that all the particles in the beam are eventually reflected. Particles can enter the region beyond the step (by barrier penetration), but they do not stay there forever and are eventually reflected.

Solution 17.3 The probability current is

$$j_x(x) = -\frac{\mathrm{i}\hbar}{2m}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right).$$

We have

$$\psi(x) = A\mathrm{e}^{\mathrm{i}kx} \quad \text{and} \quad \psi^*(x) = A^*\mathrm{e}^{-\mathrm{i}kx}$$

$$\frac{\partial\psi}{\partial x} = \mathrm{i}Ak\,\mathrm{e}^{\mathrm{i}kx} \quad \text{and} \quad \frac{\partial\psi^*}{\partial x} = -\mathrm{i}A^*k\,\mathrm{e}^{-\mathrm{i}kx}$$

so

$$\begin{aligned} j_x &= -\frac{\mathrm{i}\hbar}{2m}\left(A^*\mathrm{e}^{-\mathrm{i}kx}(\mathrm{i}Ak\,\mathrm{e}^{\mathrm{i}kx}) - A\mathrm{e}^{\mathrm{i}kx}(-\mathrm{i}A^*k\,\mathrm{e}^{-\mathrm{i}kx})\right) \\ &= -\frac{\mathrm{i}\hbar}{2m}|A|^2\left(\mathrm{i}k + \mathrm{i}k\right) \\ &= \frac{\hbar k}{m}|A|^2. \end{aligned}$$

Comment In classical terms, the answer is the probability density of the beam, multiplied by the velocity of the beam, which is appropriate for a probability current.

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